

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau



(43) International Publication Date
15 March 2001 (15.03.2001)

PCT

(10) International Publication Number
WO 01/18045 A1

(51) International Patent Classification⁷: **C07K 14/00,**
G01N 33/573

(21) International Application Number: **PCT/US00/24700**

(22) International Filing Date:
8 September 2000 (08.09.2000)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/152,753 8 September 1999 (08.09.1999) US

(71) Applicants (*for all designated States except US*):
SLOAN-KETTERING INSTITUTE FOR CANCER RESEARCH [US/US]; 1275 York Avenue, New York, NY 10021 (US). **THE TRUSTEES OF COLUMBIA UNIVERSITY IN THE CITY OF NEW YORK** [US/US]; West 116th Street and Broadway, New York, NY 10027 (US).

(72) Inventors; and

(75) Inventors/Applicants (*for US only*): **PAVLETICH, Nikola** [YU/US]; Apartment 38A, 330 East 75th Street, New York, NY 10021 (US). **FINNIN, Michael** [US/US];

504 East 63rd Street, Apt. 19S, New York, NY 10021 (US). **DONIGIAN, Jill** [US/US]; 13 Union Place, North Arlington, NJ 07031 (US). **RICHON, Victoria** [US/US]; 504 East 63rd Street, Apt. 28M, New York, NY 10021 (US). **RIFKIND, Richard, A.** [US/US]; Apt. #48A, 425 East 58th Street, New York, NY 10022 (US). **MARKS, Paul, A.** [US/US]; 7 Rossiter Road, Washington, CT 06793 (US). **BRESLOW, Ronald** [US/US]; 275 Broad Avenue, Englewood, NJ 07631 (US).

(74) Agent: **WHITE, John, P.**; Cooper & Dunham LLP, 1185 Avenue of the Americas, New York, NY 10036 (US).

(81) Designated States (*national*): CA, JP, US.

(84) Designated States (*regional*): European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE).

Published:

- *With international search report.*
- *Before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments.*

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.



WO 01/18045 A1

(54) Title: CRYSTAL STRUCTURE OF A DEACETYLASE AND INHIBITORS THEREOF

(57) Abstract: The present invention provides three-dimensional structural information from the hyperthermophilic bacterium *Aquifex aeolicus* which is a histone deacetylase-like protein (HDLP). HDLP shares 35.2% amino acid sequence identity with human histone deacetylase (HDAC1). The present invention further provides three-dimensional structural information of HDLP bound by inhibitor molecules. The three-dimensional structural information of the present invention is useful to design, isolate and screen deacetylase inhibitor compounds capable of inhibiting HDLP, HDAC family members and HDLP-related molecules. The invention also relates to nucleic acids encoding a mutant HDLP which facilitates the determination of the three-dimensional structure of HDLP in the presence of a zinc atom.

CRYSTAL STRUCTURE OF A DEACETYLASE AND INHIBITORS THEREOF

5

This application claims priority of U.S. Provisional Application No. 60/152,753, filed September 8, 1999, the contents of which are hereby incorporated by reference.

10

This invention has been made with government support under National Institutes of Health Grant No. R01 CA-65698. Accordingly, the U.S. Government may have certain rights in the invention.

15

Throughout this application, various publications are referenced by author, date and citation. The disclosures of these publications in their entireties are hereby incorporated by reference into this application in order to more fully describe the state of the art as known to those skilled therein as of the date of the invention described and claimed herein.

20

Introduction

25

The present invention relates to a histone deacetylase homologue from the hyperthermophilic bacterium *Aquifex aeolicus*, HDLP (histone deacetylase like protein; also known as AcuCl), which shares 35.2 % sequence identity with human histone deacetylase (HDAC1), that can be co-crystallized with an inhibitory ligand, and more particularly, to the detailed crystallographic data obtained from said co-crystallization which is disclosed herein. The invention also relates to methods of using the crystal structure and x-ray crystallographic coordinates of the apo-HDLP and

30

- 2 -

inhibitor-bound HDLP to design, isolate and screen compounds which bind to and inhibit the active site of HDLP and HDLP-related proteins, such as those proteins belonging to the HDAC family, including HDAC1.

5

Background of the Invention

The reversible modification of histones by acetylation is associated with changes in nucleosome conformation and chromatin structure, and plays an important role in the regulation of gene expression (reviewed in Davie and Chadee, 1998, *J. Cell Biochem. Suppl.* 30-31:203-213). The histone acetylase and deacetylase enzymes that carry out these modifications are involved in many cellular processes such as cell cycle progression and differentiation, and their deregulation is associated with several types of human cancer (reviewed in Kouzarides, 1999, *Curr. Opin. Genet. Dev.* 2:40-48; Hassig et al., 1997, *Chem. Biol.* 4:783-789; Fenrick and Heibert, 1998, *J. Cell. Biochem. Suppl.* 30-31:194-202).

20

Recently, several experimental antitumor compounds, such as trichostatin A (TSA), trapoxin, suberoylanilide hydroxamic acid (SAHA), and phenylbutyrate have been shown to act, at least in part, by inhibiting histone deacetylases. Richon et al., 1998, *Proc. Natl. Acad. Sci., USA* 95:3003-3007; Yoshida et al., 1990, *J. Biol. Chem.* 265:17174-17179; Kijima et al., 1993, *J. Biol. Chem.* 268:22429-22435. Additionally, diallyl sulfide and related molecules (Lea et al., 1999, *Int. J. Oncol.* 2:347-352), oxamflatin (Kim et al., 1999, *Oncogene* 15:2461-2470), MS-27-275, a synthetic benzamide derivative (Saito et al., 1999, *Proc. Natl. Acad. Sci.* 96:4592-4597),

30

- 3 -

butarate derivatives (Lea and Tulsyan, 1995, *Anticancer Res.* 15:879-883), FR901228 (Nokajima et al., 1998, *Exp. Cell Res.* 241:126-133), depudecin (Kwon et al., 1998, *Proc. Natl. Acad. Sci. USA* 95:3356-3361) and m-carboxysinnamic acid bishydroxamide (CBHA; Richon et al., *Proc. Natl. Acad. Sci. USA* 95:3003-3007) have been shown to inhibit histone deacetylases. In vitro, these compounds can inhibit the growth of fibroblast cells by causing cell cycle arrest in the G1 and G2 phases (Richon et al., 1996, *Proc. Natl. Acad. Sci. USA* 93:5705-5708; Kim et al., 1999, *Oncogene* 18:2461-2470; Yoshida et al., 1995, *Bioessays* 17:423-430; Yoshida & Beppu, 1988, *Exp. Cell. Res.* 177:122-131), and can lead to the terminal differentiation and loss of transforming potential of a variety of transformed cell lines. Richon et al., 1996, *Proc. Natl. Acad. Sci. USA* 93:5705-5708; Kim et al., 1999, *Oncogene* 18:2461-2470; Yoshida et al., 1987, *Cancer Res.* 47:3688-3691. In vivo, phenylbutyrate is effective in the treatment of acute promyelocytic leukemia in conjunction with retinoic acid. Warrell et al., 1998, *J. Natl. Cancer Inst.* 90:1621-1625. SAHA is effective in preventing the formation of mammary tumors in rats, and lung tumors in mice. Desai et al., 1999, *Proc. AACR* 40: abstract #2396; Cohen et al., *Cancer Res.*, submitted.

25

Histone deacetylases catalyze the removal of acetyl groups from the ϵ -amino groups of lysine residues clustered near the N-terminus of nucleosomal histones, and this process is associated with transcriptional repression (reviewed in Struhl, 1998, *Genes Dev.* 12:599-606). Deletion of the yeast histone deacetylase gene, *rpd3*, or its pharmacological

30

- 4 -

inactivation with trichostatin A reduces the transcriptional repression in a subset of promoters, such as those of Ume6-regulated genes. Kadosh & Struhl, 1998, *Mol. Cell. Biol.* 18:5121-5127. This is accompanied by the increased
5 acetylation of H4 histones in the repressed promoter and its vicinity, but has no effect on histones at promoter distal regions. Kadosh & Struhl, 1998, *Mol. Cell. Biol.* 18:5121-5127; Rundlett et al., 1998, *Nature* 392:831-835.

10 Histone deacetylases are recruited to specific promoters by associating with DNA-binding transcriptional repressors, either directly or through co-repressors that bridge the deacetylase to the transcriptional repressors. For example, the Mad and Ume6 repressors bind to the co-repressor Sin3A
15 (Laherty et al., 1997, *Cell* 89:349-356; Hassig et al., 1997, *Cell* 89:341-347; Kadosh & Struhl, 1997, *Cell* 89:365-371), and the nuclear receptors bind N-CoR and the related SMRT co-repressors. Nagy et al., 1997, *Cell* 89:373-380; Alland et al, 1997, *Nature* 387:49-55; Heinzl et al, 1997, *Nature*
20 387:43-48.

The deregulation of histone deacetylase recruitment appears to be one of the mechanisms through which these enzymes contribute to tumorigenesis. In acute promyelocytic
25 leukemia (APL), chromosomal translocations fuse the retinoic acid receptor- α (RAR α) to either PLZF or to PML. These fusion oncoproteins have aberrant transcriptional repression activity resulting, in part, through the recruitment of a co-repressor and, in turn, HDACs. Grignani et al, 1998,
30 *Nature* 391:815-818; Lin et al., 1998, *Nature* 391:811-814. Treatment of PLZF-RAR α APL cells with TSA enhances their

- 5 -

responsiveness to retinoic acid-induced differentiation. Grignani et al, 1998, *Nature* 391:815-818; Lin et al., 1998, *Nature* 391:811-814.

5 The histone deacetylases comprise a large family of proteins, conserved from yeast to man, and are divided into two related classes. Class I is characterized by human HDAC1, 2, 3 (Taunton et al., 1996, *Science* 272:408-411; Yang et al., 1996, *Proc. Natl. Acad. Sci. USA* 93:12845-12850; 10 Emiliani et al., 1998, *Proc. Natl. Acad. Sci. USA* 95:2795-2800), and yeast RPD3 (Videl & Gaber, 1991, *Mol. Cell. Biol.* 11:6317-6327), and class II by the human HDAC4, 5, 6 (Grozinger et al., 1999, *Proc. Natl. Acad. Sci. USA* 96:4868-4873; Fischle, et al., 1999, *J. Biol. Chem.* 274:11713-15 11720), and yeast HDA1 (Rundlett et al., 1996, *Proc. Natl. Acad. Sci. USA* 93:14503-14508). The two classes share a ~390 amino acid region of sequence similarity, comprising the deacetylase core, but are divergent outside this region. The histone deacetylase genes belong to an even larger 20 superfamily (Leipe & Landsman, 1997, *Nucleic Acids Res.* 25:3693-3697) that contains the prokaryotic acetoin utilization proteins (AcuC; 28.1% sequence identity to HDAC1), and the prokaryotic acetylpolymine amidohydrolases (APAH; 15.0 % sequence identity to HDAC1). The enzymatic 25 activity of AcuC is not clear, but its disruption reduces the ability of *B. subtilis* to breakdown acetoin and utilize it as a carbon source. Grundy et al., 1993, *Mol. Microbiol.* 10:259-271. APAHs catalyze the deacetylation of polyamines by cleaving a non-peptide amide bond (reviewed in Leipe & 30 Landsman, 1997, *Nucleic Acids Res.* 25:3693-3697).

- 6 -

It is useful to address the questions of how HDACs and HDAC-related proteins catalyze the deacetylation of histones and how the above-referenced compounds, particularly those compounds with antitumor activity, inhibit this activity in order to better understand the mechanism of inhibition of HDACs and to facilitate discovery of additional useful compounds which may inhibit this activity. To this end, the present invention has determined the three dimensional structure of a HDAC1-like protein from the thermophilic bacterium *Aquifex aeolicus*, herein after HDLP. The determination of the nucleic acid coding sequence of HDLP was described by Deckert et al., 1998, *Nature* 392:353-358. The encoded 375 residue protein, whose sequence was determined from the nucleic acid encoding sequence, shares 35.2% amino acid sequence identity with HDAC1, deacetylates histones *in vitro*, and is inhibited by TSA, SAHA and several other HDAC inhibitors. The determination of the three-dimensional structure of HDLP is useful in the design, identification and screening of new HDAC family inhibitory compounds which are useful for the inhibition of cell growth both *in vivo* and *in vitro*.

Summary of the Invention

In general, it is the object of the present invention to provide detailed three-dimensional structural information for a family of proteins known as histone deacetylases (HDAC), and particularly a homologue from the hyperthermophilic bacterium *Aquifex aeolicus* HDLP (histone deacetylase-like protein) which shares 35.2 % sequence identity with human histone deacetylase (HDAC1). It is also an object of the present invention to provide three-

- 7 -

dimensional structural information of an HDLP bound to an inhibitory compound.

5 In one embodiment of the invention, three-dimensional structure information is obtained from a crystal of wild-type HDLP (SEQ ID NO:1) (the nucleic acid encoding wild-type HDLP is SEQ ID NO:2). In a further embodiment of the invention, three-dimensional information is obtained from a mutant HDLP comprising two mutations (1) cysteine 75 to a
10 serine and (2) cysteine 77 to a serine (Cys75Ser/Cys77Ser double mutant; SEQ ID NO:3) (the nucleic acid encoding HDLP Cys75Ser/Cys77Ser double mutant is SEQ ID NO:4). The HDLP mutant of the present invention facilitates the determination of three-dimensional structural information of
15 HDLP bound to a zinc atom at its zinc atom-binding site.

In a preferred embodiment of the invention, the three-dimensional structural information is obtained from a co-crystal of a protein-inhibitor compound complex that
20 comprises HDLP or HDLP Cys75Ser/Cys77Ser double mutant and trichostatin A (TSA). In another preferred embodiment of the invention the three-dimensional structural information is obtained from a co-crystal of a protein-inhibitor compound complex that comprises HDLP or HDLP
25 Cys75Ser/Cys77Ser double mutant and suberoylanilide hydroxamic acid (SAHA). Any HDLP or HDLP-related protein (e.g. HDAC) inhibitor compound that may be co-crystallized with HDLP may be used to form a co-crystal of the present invention.

30

The protein crystals and protein-inhibitory complex co-crystals of the present invention diffract to a high

- 8 -

resolution limit of at least equal to or greater than 4 angstrom (Å). In a preferred embodiment, the protein crystals and protein-inhibitory complex co-crystals of the present invention diffract to a high resolution limit of
5 greater than 2.5 Å.

A crystal of the present invention may take a variety of forms, all of which are contemplated by the present invention. In a preferred embodiment, the crystal has a
10 space group of C2 with one molecule in the asymmetric unit and with unit dimensions of $a = 51.4 \text{ Å}$, $b = 93.8 \text{ Å}$, $c = 78.7 \text{ Å}$ and $\beta = 96.9^\circ$ (see, e.g., Example 2, below). In another preferred embodiment, the crystal has a space group of P2₁2₁2₁ with two molecules in the asymmetric unit and with
15 unit dimensions of $a = 53.4 \text{ Å}$, $b = 94.4 \text{ Å}$, $c = 156.3 \text{ Å}$ (see, e.g., Example 2, below). The HDLP structure comprises a parallel β sheet with α helices packing against both faces. At one end of the β sheet, the HDLP has a narrow, tube-like pocket formed by several well-ordered loops. The walls of
20 the pocket are lined with hydrophobic residues and there is a zinc binding site and several polar side chains at the bottom of the pocket. The inhibitory compounds of the present invention bind in the pocket.

25 The three-dimensional structural information obtained from crystals of HDLP, HDLP Cys75Ser/Cys77Ser double mutant, HDLP Cys75Ser/Cys77Ser double mutant comprising a zinc atom, HDLP comprising an inhibitory compound such as TSA or SAHA, and HDLP Cys75Ser/Cys77Ser double mutant comprising an inhibitor
30 compound such as TSA or SAHA may be employed to solve the structure of any HDLP-related protein (e.g. HDAC) crystal,

- 9 -

or any mutant HDLP-related protein and particularly any wild type or mutant of HDLP-related protein complexed with a ligand, including a substrate or inhibitor compound. If the crystals are in a different space group than the known structure, molecular replacement may be employed to solve
5 the structure, or if the crystals are in the same space group, refinement and difference fourier methods may be employed. The structure of HDLP-related proteins (e.g. HDAC1) comprise no greater than a 2.0 Å root mean square deviation (rmsd) in the positions of the C α atoms for at
10 least 50% or more of the amino acids of the full-length HDLP structure.

The present invention also provides a nucleic acid molecule
15 encoding an HDLP Cys75Ser/Cys77Ser double mutant having the amino acid sequence of SEQ ID NO:3 and the nucleic acid sequence of SEQ ID NO:4. It is also contemplated by the invention that mutations be made in HDLP-related proteins at cysteine residues, as with the Cys75Ser/Cys77Ser double
20 mutant, in order to facilitate the determination of the structure of said proteins bound to a zinc atom. Additionally, the present invention provides expression vectors which comprise the nucleic acid molecule encoding an HDLP Cys75Ser/Cys77Ser double mutant encoded by the sequence
25 represented by SEQ ID NO:4 operatively linked to expression control sequences.

It is another object of the present invention to provide methods for the design, identification and screening of
30 potential inhibitor compounds of the HDLP/HDAC family. In a preferred embodiment the method for the rational design,

- 10 -

identification and screening of potential inhibitor compounds for HDLP and HDLP-related proteins (e.g. HDACs) comprising deacetylase activity comprises the steps of: (a) using a three-dimensional structure of an HDLP as defined by the atomic coordinates of the present invention; (b) employing said three-dimensional structure to design or select said potential inhibitor compound; (c) synthesizing and/or selecting said potential inhibitor; (d) contacting said potential inhibitor compound with said enzyme in the presence of acetylated substrate; and (e) determining the percent inhibition of deacetylase activity to determine the inhibitory activity of said potential inhibitor compound. In a further preferred embodiment, the binding properties of said rationally designed inhibitory compound may be determined by a method comprising the steps of: (a) forming a complex comprising said inhibitory compound and HDLP or a HDLP-related protein, (b) co-crystallizing said inhibitory compound-HDLP complex; (c) determining said three-dimensional structure of said co-crystal through molecular replacement or refinement and difference fourier with the molecular coordinates of HDLP as defined by the present invention; and (d) analyzing the three-dimensional structure to determine the binding characteristics of said potential inhibitor compound.

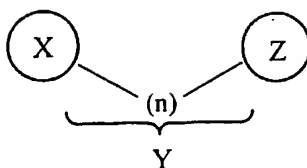
25

It is a further object of the present invention to identify a defined class of HDLP/HDAC family inhibitor compounds. The HDLP/HDAC family inhibitor compounds of the present invention are represented by formula (I):

30

- 11 -

(I)



5

wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of proline and leucine; Y comprises an aliphatic chain group which binds to at least one amino acid selected from the group consisting of leucine, phenylalanine and glycine; and Z comprises an active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and may further bind to a zinc atom.

15

20

25

30

Brief Description of the Drawings

Figure 1 is a table listing the statistics from the X-ray crystallographic analysis of a HDLP crystal, a HDLP-TSA co-crystal, and a HDLP-SAHA co-crystal.

5

Figure 2 shows an alignment of various HDAC homologues with percent sequence identity depicted.

Figure 3 shows a graph indicating the histone deacetylase activity of HDLP and HDAC1 and the inhibition of HDLP and HDAC1 by the inhibitors TSA and HC-toxin.

10

Figure 4 shows (A & B) a schematic representation of the HDLP-Zn²⁺-TSA complex in two approximately orthogonal views, (C) a topology diagram of HDLP indicating the regions of homology with HDAC1, and (D) a close-up schematic representation of the HDLP-Zn²⁺-SAHA complex.

15

Figure 5 shows (A) a schematic representation of a slice through a surface representation of HDLP with the pocket internal cavities and position of the β sheet indicated, (B) a schematic representation of a close-up view of the active site looking down into the pocket in an orientation similar to Figure 4B.

20

25

Figure 6 shows (A) a space-filling representation of TSA in the active site pocket, (B) a closeup stereo view of the structure of the HDLP-Zn²⁺-TSA complex in a similar orientation to Figure 4B, and (C) a schematic representation of the HDLP-TSA interactions.

30

- 13 -

Figure 7 shows (A) a schematic representation of the regions of homology shared between HDLP and HDAC1 in an orientation similar to that of Figure 4A, and (B) a detailed schematic representation of the homology shared in the pocket and internal cavity between HDLP and HDAC1 in an orientation similar to that of Figure 4B.

Figure 8 shows a schematic representation of the proposed catalytic mechanism for the deacetylation of acetylated lysine.

Figure 9 shows a schematic representation of a space filling diagram showing the conserved amino acids in the active site and nearby grooves.

Figure 10 is the nucleic acid sequence of HDLP from *Aquifex aeolicus* (SEQ ID NO. 2).

Figure 11 is the amino acid sequence of full length HDLP from *Aquifex aeolicus* (SEQ ID NO. 1).

Figure 12 is the nucleic acid sequence of the HDLP active site mutant Tyr297Phe (SEQ ID NO. 6).

Figure 13 is the amino acid sequence of the HDLP active site mutant Tyr297Phe (SEQ ID NO. 5).

Figure 14 is the nucleic acid sequence of a double mutant of HDLP from *Aquifex aeolicus* comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO. 4).

- 14 -

Figure 15 is the amino acid sequence of a double mutant of HDLP from *Aquifex aeolicus* comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO. 3).

5 Figure 16-1 to 16-49 lists the atomic structure coordinates for HDLP as derived by X-ray diffraction from a crystal of HDLP.

10 Figure 17-1 to 17-49 lists the atomic structure coordinates for HDLP Cys75Ser/Cys77Ser double mutant comprising a zinc atom in the active site as derived by X-ray diffraction from a crystal of the HDLP Cys75Ser/Cys77Ser double mutant.

15 Figure 18-1 to 18-99 lists the atomic structure coordinates for HDLP Cys75Ser/Cys77Ser double mutant as derived by X-ray diffraction from a co-crystal of HDLP complexed with TSA.

20 Figure 19-1 to 19-48 lists the atomic structure coordinates for HDLP Cys75Ser/Cys77Ser double mutant as derived by X-ray diffraction from a co-crystal of HDLP complexed with SAHA.

25

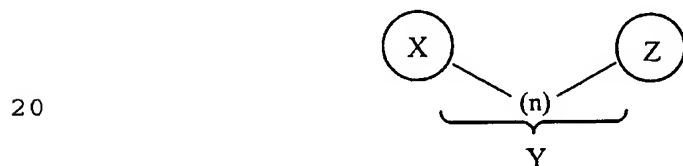
30

Detailed Description of the Invention

The present invention provides crystals of a histone deacetylase (HDAC) homologue grown in the presence and absence of a compound capable of inhibiting the histone deacetylase activity of said HDAC homologue. As referred to
5 herein, a HDAC homologue (as well as a HDLP-related protein) is any protein molecule having (a) greater than 15% sequence identity to over the 375 amino acid residues of HDLP; (b) having no more than twenty insertions or deletions for a
10 total of no more than 100 amino acids; and (c) deacetylase activity. Sequence identity is calculated by the program DNASTar™ using the identity matrix weighing scheme clustal method (DNASTar program, Madison, WI).

15 A HDLP/HDAC inhibitor compound, as used herein, refers to any compound represented by Formula (I):

(I)



wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of tyrosine, proline and leucine; Y comprises an aliphatic chain group
25 from about 5 to about 10 Å, preferably 7 Å, which binds to at least one amino acid selected from the group consisting of phenylalanine and glycine; and Z comprises a active site binding group which binds to at least one amino acid
30 selected from the group consisting of aspartic acid, tyrosine and histidine and which may further bind to a zinc atom. The HDAC inhibitory compounds of the present

- 16 -

invention can inhibit greater than 50% of the histone deacetylase activity of a HDAC homologue or a HDLP-related protein.

5 To grow the crystals of the present invention, the HDAC and HDAC-inhibitory compound complex are purified to greater than 80% total protein and more preferably purified to greater than 90% total protein. For expression and purification purposes, the full-length HDLP (Genbank
10 accession number AE000719) may be subcloned from *Aquifex aeolicus* chromosomal DNA preparation by the polymerase chain reaction (PCR) and inserted into an expression vector.

A large number of vector-host systems known in the art may
15 be used. Possible vectors include, but are not limited to, plasmids or modified viruses, but the vector system must be compatible with the host cell used. Examples of vectors include *E. coli* bacteriophages such as lambda derivatives, or plasmids such as pBR322 derivatives or pUC plasmid
20 derivatives, e.g., pGEX vectors (Amersham-Pharmacia, Piscataway, New Jersey), pET vectors (Novagen, Madison, WI), pmal-c vectors (Amersham-Pharmacia, Piscataway, New Jersey), pFLAG vectors (Chiang and Roeder, 1993, *Pept. Res.* 6:62-64), baculovirus vectors (Invitrogen, Carlsbad, CA; Pharmingen,
25 San Diego, CA), etc. The insertion into a cloning vector can, for example, be accomplished by ligating the DNA fragment into a cloning vector which has complementary cohesive termini, by blunt end ligation if no complementary cohesive termini are available or by through nucleotide
30 linkers using techniques standard in the art. E.g., Ausubel et al. (eds.), *Current Protocols in Molecular*

- 17 -

Biology, (1992). Recombinant vectors comprising the nucleic acid of interest may then be introduced into a host cell compatible with the vector (e.g. *E. coli*, insect cells, mammalian cells, etc.) via transformation, transfection, 5 infection, electroporation, etc. The nucleic acid may also be placed in a shuttle vector which may be cloned and propagated to large quantities in bacteria and then introduced into a eukaryotic cell host for expression. The vector systems of the present invention may provide 10 expression control sequences and may allow for the expression of proteins *in vitro*.

In a preferred embodiment, the full length HDLP (SEQ ID NO:2) is subcloned from *Aquifex aeolicus* chromosomal DNA 15 preparation into pGEX4T3 (Amersham-Pharmacia, Piscataway, New Jersey). In order to construct a double mutant comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO:4), and to construct the HDLP active site mutant Tyr297Phe (SEQ ID NO:5 and SEQ ID NO:6), PCR site directed mutagenesis may 20 be employed with verification by DNA sequencing by methods known to those skilled in the art (see, e.g., Example 1 below). The mutants of the present invention may be subcloned into a suitable expression vector and introduced into a host cell for protein production, as described above.

25 The HDLP nucleic acids of the present invention may be subcloned into an expression vector to create an expression construct such that the resultant HDLP molecule which is produced comprises a fusion protein wherein said fusion 30 protein comprises a tag for ease of purification. As referred to herein, a "tag" is any additional amino acids

- 18 -

which are provided in a protein either c-terminally, n-terminally or internally for the ease of purification, for the improvement of production or for any other purpose which may facilitate the goals of the present invention (e.g. to achieve higher levels of production and/or purification). Such tags include tags known to those skilled in the art to be useful in purification such as, but not limited to, his tag, glutathione-s-transferase tag, flag tag, mbp (maltose binding protein) tag, etc. In a preferred embodiment, the wild-type and mutant HDLPs of the present invention are tagged with glutathione-s-transferase (see Example 1 below). In another preferred embodiment, HDAC1 is flag tagged (see Example 1 below). Such tagged proteins may also be engineered to comprise a cleavage site, such as a thrombin, enterokinase or factor X cleavage site, for ease of removal of the tag before, during or after purification. Vector systems which provide a tag and a cleavage site for removal of the tag are particularly useful to make the expression constructs of the present invention.

The tagged HDLPs and HDACs of the present invention may be purified by immuno-affinity or conventional chromatography, including but not limited to, chromatography employing the following: glutathione-sepharose™ (Amersham-Pharmacia, Piscataway, New Jersey) or an equivalent resin, nickel or cobalt-purification resins, anion exchange chromatography, cation exchange chromatography, hydrophobic resins, gel filtration, antFLAG epitope resin, reverse phase chromatography, etc. After purification, the HDLP and HDLP-inhibitor compound complex may be concentrated to greater than 1 mg/ml for crystallization purposes. In a preferred embodiment HDLP and HDLP-inhibitor complexes are

- 19 -

concentrated to greater than 10 mg/ml for crystallization and in a particularly preferred embodiment, HDLP and HDLP-inhibitor complexes are concentrated to greater than 20 mg/ml.

5

In order to determine whether the purified HDLPs of the present invention demonstrate histone deacetylase activity, the purified HDLPs and also any HDLP-related protein may be assayed by any method known to those skilled in the art for the determination of said activity. In a preferred embodiment, the purified HDLPs of the present invention are incubated in the presence of [³H]acetyl-labeled histone substrate (Carmen et al., 1996, *J. Biol. Chem.* 271:15837-15844) in a buffer suitable for detection of histone deacetylase activity (see Example 3 below); stopping the reaction; extracting the released acetate and measuring said released acetate, as described by Henzel et al. (*J. Biol. Chem.* 266:21936-21942 (1991); Example 3 below). In a preferred embodiment, the HDLPs of the present invention are incubated in the presence of ZnCl₂ in order to obtain histone deacetylase activity therefrom (Example 3 below).

In another embodiment, the crystals of the present invention comprise purified wild-type HDLP (SEQ ID NO:1) and are grown at room temperature by the hanging-drop vapor-diffusion method from a crystallization solution comprising one or more precipitants selected from the group consisting of isopropanol, polyethylene glycol, and tert butanol (see Example 2 below). The crystallization solution may further comprise one or more salts including salts selected from the group consisting of NaCl and KCl, and one or more buffers

30

- 20 -

including buffers selected from the group consisting of Tris (tris(hydroxymethyl)aminomethane and bis-tris propane-Cl (1,3-bis[tris(hydroxymethyl)methyl-amino] propane) (see Example 2 below). The pH of the crystallization solution is preferably between pH 5 to 9, although other pH values are also contemplated by the present invention (see Example 2 below).

Any crystallization technique known to those skilled in the art may be employed to obtain the crystals of the present invention, including, but not limited to, batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and micro dialysis. Seeding of the crystals in some instances may be required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used.

The crystals of the present invention may form in the space group C2 with one molecule in the asymmetric unit and with unit dimensions of $a = 51.4 \text{ \AA}$, $b = 93.8 \text{ \AA}$, $c = 78.7 \text{ \AA}$ and $\beta = 96.9^\circ$ (see Example 2 below). The crystals of the present invention may also form in the space group $P2_12_12_1$ with two molecules in the asymmetric unit and with unit dimensions of $a = 53.4 \text{ \AA}$, $b = 94.4 \text{ \AA}$, $c = 156.3 \text{ \AA}$ (see Example 2 below). However, the present invention contemplates crystals which form in any space group including, but not limited to, C2, $P2_1$, $P2_12_12_1$, $P3_12_1$, $P4_32_12_1$, and $C222_1$. The crystals diffract to a resolution greater than 4 \AA , preferably greater than 2.5 \AA .

30

To collect diffraction data from the crystals of the present

- 21 -

invention, the crystals may be flash-frozen in the crystallization buffer employed for the growth of said crystals, however with preferably higher precipitant concentration (see, e.g., Example 2 below). For example, but not by way of limitation, if the precipitant used was 28% PEG 1500, the crystals may be flash frozen in the same crystallization solution employed for said crystal growth wherein the concentration of the precipitant is increased to 35% (see Example 2 below). If the precipitant is not a sufficient cryoprotectant (i.e. a glass is not formed upon flash-freezing), cryoprotectants (e.g. glycerol, low molecular weight PEGs, alcohols, etc) may be added to the solution in order to achieve glass formation upon flash-freezing, providing the cryoprotectant is compatible with preserving the integrity of the crystals. The flash-frozen crystals are maintained at a temperature of less than -110°C and preferably less than -150°C during the collection of the crystallographic data by X-ray diffraction. The X-ray diffraction data may be processed with DENZO and SCALEPACK (Otwinowski & Minor, 1997, *Method Ensemble*. 276:307-326) but any method known to those skilled in the art may be used to process the X-ray diffraction data.

In order to determine the atomic structure of HDLP according to the present invention, multiple isomorphous replacement (MIR) analysis, model building and refinement may be performed. For MIR analysis, the crystals may be soaked in heavy-atoms to produce heavy atom derivatives necessary for MIR analysis. As used herein, heavy atom derivative or derivitization refers to the method of producing a chemically modified form of a protein or protein complex

- 22 -

crystal wherein said protein is specifically bound to a heavy atom within the crystal. In practice a crystal is soaked in a solution containing heavy metal atoms or salts, or organometallic compounds, e.g., lead chloride, gold cyanide, thimerosal, lead acetate, uranyl acetate, mercury chloride, gold chloride, etc, which can diffuse through the crystal and bind specifically to the protein. The location(s) of the bound heavy metal atom(s) or salts can be determined by X-ray diffraction analysis of the soaked crystal. This information is used to generate MIR phase information which is used to construct the three-dimensional structure of the crystallized HDLPs and HDLP-related proteins of the present invention. In a preferred embodiment, the heavy atoms comprise thimerosal, $\text{KAu}(\text{CN})_2$ and $\text{Pb}(\text{Me})_3\text{OAc}$ (see Example 2 below). The MIR phases may be calculated by any program known to those skilled in the art and preferably with the program MLPHARE (The CCP4 suite: Programs for computational crystallography, 1994, *Acta Crystallogr. D.* 50:760-763) and may also use the anomalous diffraction signal from the thimerosal derivative. In a preferred embodiment, the MIR phases were calculated at 2.5 Å and have a mean figure of merit of 0.55 (see Figure 19 and Example 2 below). The phases may be improved where necessary by solvent flattening by methods known to those skilled in the art including, but not limited to, through the use of the program DM (The CCP4 suite: Programs for computational crystallography, 1994, *Acta Crystallogr. D* 50:760-763).

Thereafter, an initial model of the three-dimensional structure may be built using the program O (Jones et al.,

1991, *Acta Crystallogr. A* 47:110-119). The interpretation and building of the structure may be further facilitated by use of the program CNS (Brunger et al., 1998, *Acta Crystallogr. D* 54:905-921).

5

For the determination of the HDLP-inhibitor compound complex structure, if the space group of the HDLP-inhibitor compound complex crystal is different, molecular replacement may be employed using a known structure of apo-HDLP (as referred to herein, apo-HDLP or apo-HDAC is the enzyme which is not complexed with an inhibitor compound) or any known HDLP/inhibitor complex structure whose structure may be determined as described above and below in Example 2. If the space group of the HDLP-inhibitor compound crystals is the same, then rigid body refinement and difference fourier may be employed to solve the structure using a known structure of apo-HDLP (as referred to herein, apo-HDLP or apo-HDAC is the enzyme which is not complexed with an inhibitor compound) or any known HDLP/inhibitor complex structure.

20

The term "molecular replacement" refers to a method that involves generating a preliminary model of the three-dimensional structure of the HDLP crystals of the present invention whose structure coordinates are unknown prior to the employment of molecular replacement. Molecular replacement is achieved by orienting and positioning a molecule whose structure coordinates are known (in this case the previously determined apo-HDLP) within the unit cell as defined by the X-ray diffraction pattern obtained from an HDLP or HDLP-related protein crystal whose structure is

30

- 24 -

unknown so as to best account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of several forms of refinement to provide a final, accurate structure.

Any method known to the skilled artisan may be employed to determine the structure by molecular replacement. For example, the program AMORE (The CCP4 suite: Programs for computational crystallography, 1994, *Acta Crystallogr. D.* 50:760-763) may be employed to determine the structure of an unknown histone deacetylase +/- an inhibitor by molecular replacement using the apo-HDLP coordinates (Figure 16). For the structure determination of the inhibitory compound TSA, the structure of TSA was obtained from the Cambridge Structural Database (Refcode TRCHST, << <http://www.ccdc.cam.ac.uk> >>) may be employed to define the stereochemical restraints used in the refinement with the program CNS (Brunger et al., 1998, *Acta Crystallogr. D* 54:905-921).

The three-dimensional structural information and the atomic coordinates associated with said structural information of HDLP are useful for solving the structure of crystallized proteins which belong to the HDAC family by molecular replacement. Similarly, any structure of a crystallized protein which is thought to be similar in structure based on function or sequence similarity or identity to HDLP may be solved by molecular replacement with the HDLP structural

- 25 -

information of the present invention. The structure of HDLP-related proteins as determined by molecular replacement as described above and in Example 2 below, comprise a root mean square deviation (rmsd) of no greater than 2.0 Å in the positions of Cα atoms for at least 50% or more of the amino acids of the structure over the 375 residues of full-length HDLP. Such a rmsd may be expected based on the amino acid sequence identity. Chothia & Lesk, 1986, *Embo J.* 5:823-826.

The refined three-dimensional HDLP structures of the present invention, specifically apo-HDLP, Cys75Ser/Cys77Ser double mutant HDLP comprising a zinc atom in the active site, HDLP/TSA complex comprising a zinc atom in the active site, and HDLP/SAHA complex comprising a zinc atom in the active site, are represented by the atomic coordinates set forth in Figures 16 to 19 respectively. The refined model for apo-HDLP comprising amino acids 1-375 consists of wild-type HDLP residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered and was determined to a resolution of 1.8 Å. Similarly, the refined model for Cys75Ser/Cys77Ser double mutant HDLP comprising a zinc atom in the active site also consists of residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered and was determined to a resolution of 2.0 Å. The refined model for the HDLP/TSA complex comprising a zinc atom in the active site consists of the Cys75Ser/Cys77Ser double mutant HDLP residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered, has TSA in the binding pocket and was determined to a resolution of 2.1 Å. The HDLP/SAHA complex is similar to the HDLP/TSA complex but has SAHA in the binding pocket and was determined to a resolution of 2.5 Å.

- 26 -

For the purposes of further describing the structure of HDLP and HDLP-related proteins, including, but not limited to, HDACs, from the data obtained from the HDLP crystals of the present invention, the definition of the following terms is provided:

The term " β sheet" refers to two or more polypeptide chains (or β strands) that run alongside each other and are linked in a regular manner by hydrogen bonds between the main chain C=O and N-H groups. Therefore all hydrogen bonds in a beta-sheet are between different segments of polypeptide. Most β -sheets in proteins are all-parallel (protein interiors) or all-antiparallel (one side facing solvent, the other facing the hydrophobic core). Hydrogen bonds in antiparallel sheets are perpendicular to the chain direction and spaced evenly as pairs between strands. Hydrogen bonds in parallel sheets are slanted with respect to the chain direction and spaced evenly between strands.

The term " α helix" refers to the most abundant helical conformation found in globular proteins. The average length of an α helix is 10 residues. In an α helix, all amide protons point toward the N-terminus and all carbonyl oxygens point toward the C-terminus. The repeating nature of the phi, psi pairs ensure this orientation. Hydrogen bonds within an α helix also display a repeating pattern in which the backbone C=O of residue X (wherein X refers to any amino acid) hydrogen bonds to the backbone HN of residue X+4. The α helix is a coiled structure characterized by 3.6 residues per turn, and translating along its axis 1.5 Å per amino acid. Thus the pitch is 3.6x1.5 or 5.4 Å. The screw sense of alpha helices is always right-handed.

- 27 -

The term "loop" refers to any other conformation of amino acids (i.e. not a helix, strand or sheet). Additionally, a loop may contain bond interactions between amino acid side chains, but not in a repetitive, regular fashion.

5

Amino acid residues in peptides shall herein after be abbreviated as follows: Phenylalanine is Phe or F; Leucine is Leu or L; Isoleucine is Ile or I; Methionine is Met or M; Valine is Val or V; Serine is Ser or S; Proline is Pro or P; Threonine is Thr or T; Alanine is Ala or A; Tyrosine is Tyr or Y; Histidine is His or H; Glutamine is Gln or Q; Asparagine is Asn or N; Lysine is Lys or K; Aspartic Acid is Asp or D; Glutamic Acid is Glu or E; Cysteine is Cys or C; Tryptophan is Trp or W; Arginine is Arg or R; and Glycine is Gly or G. For further description of amino acids, please refer to *Proteins: Structure and Molecular Properties* by Creighton, T.E., W.H. Freeman & Co., New York 1983.

The term "positively charged amino acid" refers to any amino acid having a positively charged side chain under normal physiological conditions. Examples of positively charged amino acids are Arg, Lys and His. The term "negatively charged amino acid" refers to any amino acid having a negatively charged side chain under normal physiological conditions. Examples of negatively charged amino acids are Asp and Glu. The term "hydrophobic amino acid" refers to any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples of hydrophobic amino acids are Ala, Leu, Ile, Gly, Val, Pro, Phe, Trp and Met. The term "hydrophilic amino acid" refers to any amino acid having an uncharged, polar side chain that is

- 28 -

relatively soluble in water. Examples of hydrophilic amino acids are Ser, Thr, Tyr, Asp, Gln, and Cys. The term "aromatic amino acid" refers to any amino acid comprising a ring structure. Examples of aromatic amino acids are His, Phe, Trp and Tyr.

The term "charge relay system" refers to a His-Asp arrangement as described by Fersht & Sperling, 1973, *J. Mol. Biol.* 74:137-149; Blow et al., 1969, *Nature* 221:337-340.

10

The information obtained from the three-dimensional structures of the present invention reveal that HDLP has a single-domain structure that belongs to the open α/β class of folds (see, e.g., Branden, 1980, *Q. Rev. Biophys.* 13:317-38). Two orthogonal views of the overall three-dimensional structure of HDLP are depicted in Figure 4A and 4B. The HDLP structure has a central eight-stranded parallel β sheet (strands arranged as $\beta 2-\beta 1-\beta 3-\beta 8-\beta 7-\beta 4-\beta 5-\beta 6$), and sixteen α helices (labeled $\alpha 1$ through $\alpha 16$ respectively). See Figure 4C. Four of the helices pack on either face of the β sheet ($\alpha 7$, $\alpha 8$, $\alpha 9$, $\alpha 10$ and $\alpha 11$, $\alpha 12$, $\alpha 13$, $\alpha 14$) forming the core α/β structure characteristic of this class of folds. Most of the remaining eight helices are positioned near one side of the β sheet, near strands $\beta 2-\beta 1-\beta 3-\beta 8$. Large, well defined loops (Loops L1-L7; Figure 4C) originate from the C-terminal ends of the β -strands. The extra helices and the large L1-L7 loops are associated with a significant extension of the structure beyond the core α/β motif. This extension of the structure gives rise to two prominent architectural features: a deep, narrow pocket and an internal cavity adjacent to the pocket. These

30

- 29 -

two architectural features comprise the active site (see Figure 5A). The structure of HDLP-related proteins (e.g. HDACs) may also comprise the conserved α/β structure characteristic.

5

The term "active site" comprises any or all of the following sites in HDLP, the substrate binding site, the site where the cleavage of an acetyl group from a substrate occurs or the site where an inhibitor of the HDAC family or, more particularly, HDLP binds. The active site, as referred to herein, comprises Asp166, Asp258, His170, Tyr297, His131, His132, Asp168, Asp173, Phe141, Phe198, Leu265, Pro22 and Gly140, and also a metal bound at the bottom of the pocket by Asp173, Asp168 and His defined by the coordinates listed in Figures 16 to 19 with an rmsd of 2.0 Å. The metal which binds at the bottom of the pocket will be a divalent cation selected from the group consisting of zinc, cobalt or manganese.

20 The deep narrow pocket has a tube-like shape with a depth of ~ 11 Å. The pocket opening constricts half way down to ~ 4.5 by 5.5 Å, and becomes wider at the bottom (see Figure 5A). The pocket and its immediate surroundings are made up of loops L1 through L7.

25

The walls of the pocket are covered with side chains of hydrophobic and aromatic residues (Pro22, Tyr91 near the entrance; and Gly140, Phe141, Phe 198, Leu265 and Tyr297 further down; Figure 5B). For numbering of amino acids please refer to SEQ ID NO:1. Of particular interest are Phe141 and Phe198, whose phenyl groups face each other in

30

- 30 -

parallel at a distance of 7.5 Å, marking the most slender portion of the pocket (see Figure 5B). Of particular interest is that only one pocket residue differs in HDAC1 when the sequences are aligned (alignment may be accomplished using DNASTar™ MegAlign™ program, Madison, WI), this residue is Glu98 of HDAC1 which is Tyr91 in HDLP. The structure reveals that this residue in HDLP is mostly solvent exposed.

10 Near the bottom of the pocket of the active site at its narrowest point, is located a zinc ion (see Figure 6A). In order to obtain the zinc in the structure, the crystals may be soaked in zinc (e.g. ZnCl₂) or co-crystallized in the presence of zinc. The zinc ion is coordinated by Asp168
15 (Oδ1, 2.1 Å), His170 (Nδ1, 2.1 Å), Asp258 (Oδ1, 1.9 Å) and a water molecule (2.5 Å). See Figure 5B and 6B. The amino acid residues that coordinate zinc are arranged in a tetrahedral geometry, but the position of the water molecule, which is also hydrogen bonded to His131, deviates
20 from this geometry by ~25°.

In addition to the zinc ligands, the bottom of the pocket contains two histidine (His131 and His132), two aspartic acids (Asp166 and Asp173) and a tyrosine (Tyr297). See
25 Figure 5B and 10B. Each of the histidines makes a hydrogen bond through its Nδ1 to an aspartic acid carboxylate oxygen, with the oxygen located in the plane of the imidazole ring (Figure 5B). This His-Asp arrangement is characteristic of the charge relay system present in the active sites of
30 serine proteases, where it serves to polarize the imidazole Ne and increase its basicity. Fersht & Sperling, 1973, J.

- 31 -

Mol. Biol. 74:137-149; Blow et al., 1969, *Nature* 221:337-340.

5 The Asp166-His131 charge pair relay (hereafter referred to as "buried charged relay") is positioned even deeper in the pocket and more buried compared to the Asp173-His132 charge relay (hereafter referred to as "exposed charge relay") which is partially solvent exposed. The buried charge relay makes a hydrogen bond (2.6 Å) to the zinc-bound water
10 molecule referred to above, and this hydrogen bond could contribute to the deviation of the water-zinc coordination from ideal geometry (Figure 5B). The exposed charge relay is directed to a point ~ 2.5 Å away from the water molecule and closer to the surface.

15 Tyr 297 is positioned next to the zinc, opposite from where the two charge relay systems are located. The Tyr hydroxyl group lies 4.4 Å away from the zinc atom and has no interactions with the rest of the protein (Figure 5B). Next
20 to Tyr297, there is an opening in the pocket wall, which leads to the adjacent internal cavity.

The floor of the internal cavity is made up of portions of the L3 and L7 loops as they emerge from the β strands, and
25 the roof is made up by the α1-L1-α2 segment. The L1 loop appears more flexible than other loops in the structure. This may allow the transient exchange of the cavity contents with the bulk solvent.

30 The cavity is lined primarily with hydrophobic residues and is particularly rich in glycine residues (Ala127, Gly128, Gly129, Met130, and Phe141 of L3; Gly293, Gly294, Gly295 and

- 32 -

Gly296 of L7; and Tyr17, Pro22 and Leu23 of L1). There are only two charged residues in the cavity (Arg27 and His 21) and these are contributed by the L1 loop.

5 The cavity may provide space for the diffusion of the acetate product away from the catalytic center, which may otherwise be crowded and shielded during deacetylation from the solvent when the substrate is bound. Such a role for the cavity is supported by the observation that the cavity
10 contains three water and two isopropanol molecules (from the crystallization buffer) in the 1.8 Å apo-protein structure. The cavity may also bind another cofactor, in addition to zinc, for the facilitation of the enzymatic activity of the HDLP. A proposed catalytic mechanism for deacetylation is
15 provided in Figure 8.

The structure of HDLP as defined by the present invention, in conjunction with the HDAC1 sequence homology, shows that the 375-amino acid HDLP protein corresponds to the histone
20 deacetylase catalytic core which is conserved across the HDAC family (see Figure 2). The 35.2% HDLP-HDAC1 sequence identity predicts structural similarity with a rmsd in C α positions of ~ 1.5 Å. Chothia and Lesk describe the relation between the divergence of sequence and the
25 structure of proteins in *Embo J.* 5:823-826 (1986). The 40-residue C-terminus of HDLP is likely to have a divergent structure since this region has lower homology to HDAC1, although the α 16 helix in this region is part of the conserved open α/β core fold and HDAC1 is likely to comprise
30 a similar helix. However divergent this C-terminal region may be, this region is outside the active site and is likely to not effect the structure of the active site. Beyond the

- 33 -

C-terminus of the histone deacetylase catalytic core, HDAC family members are divergent in length and sequence. In the HDAC family, this region (amino acid residues ~390-482) is highly polar, populated with acidic residues, and is likely to be flexible or loosely folded.

The HDLP-HDAC homology maps primarily to the hydrophobic core and to the L1-L7 loops, with portions of the loops that make up the pocket and adjacent cavity having the highest level of amino acid residue sequence conservation (Figure 9A and 9B). Specifically, all of the polar residues in the active site (the zinc ligands, the two charge relay systems, and Tyr297) and the hydrophobic residues that make up the walls of the pocket (Gly140, Phe141, Phe198 and Leu265) are identical. Among the residues that make up the internal cavity, the ones closest to the active site are either identical or conservatively substituted (for example, Leu23 → Met and Met130 → Leu). Surface residues around the pocket are conserved to a lesser extent, but are still above 35% average sequence identity.

The information obtained from the inhibitor-bound HDLP complex crystal structures of the present invention reveal detailed information which is useful in the design, isolation, screening and determination of potential inhibitor compounds which may inhibit HDLP/HDAC family members. As described above, the HDLP structure consists of a parallel β sheet with α helices packing against both faces (Figure 4A, 4B, and 4C). At one end of the β sheet, 7 loops (L1-L7) form a narrow, tube-like pocket which are lined with hydrophobic residues and which comprise a zinc binding site, several polar side chains, including two Asp-His charge

- 34 -

relay systems. Mutation of the zinc ligands and other polar residues at the pocket bottom reduces or eliminates the catalytic activity.

5 The present inventors found that mutation at the Tyr297Phe site reduced activity. See also, Hassig et al., 1998, *Proc. Natl. Acad. Sci. USA* 95:3519-3524; Kadosh & Struhl, 1998, *Genes Dev.* 12:797-805. The elimination of activity by mutation of these residues indicates that this region is the
10 enzyme active site. Adjacent to the active site, there is an internal cavity that may provide space for the diffusion of the acetate reaction product. Homology at the active site between HDLP and HDAC1, as described above, indicates that they share structural and functional homology.

15 The inhibitor compound, trichostatin A (TSA) (Tsuji et al., 1976, *J. Antibiotics* 29:1-6) binds HDLP by inserting its long aliphatic chain, which has a hydroxamic acid group at one end, into the pocket (Figure 6A, 6B and 6C). The
20 aliphatic chain makes multiple contacts in the well-like, hydrophobic portion of the pocket. The hydroxamic acid reaches the polar bottom of the pocket, where it coordinates the zinc in a bidentate fashion and also forms hydrogen bonds with the polar residues in the active site, including
25 the two charge relay system histidines. The aromatic dimethylamino-phenyl group at the other end of the TSA chain makes contacts at the pocket entrance and serves to cap it. The amino acid residues of HDLP which contact TSA are conserved in HDAC, indicating that TSA binds and inhibits
30 HDAC in a similar fashion to HDLP.

- 35 -

In the complex, the hydroxamic acid, most of the aliphatic chain and part of the dimethylamino-phenyl group of TSA are buried (60% of TSA's surface area; Figure 6A). The hydroxamic acid group binds the zinc in a bidentate fashion forming bonds through its carbonyl (2.4 Å) and hydroxyl groups (2.2 Å) resulting in a penta-coordinated Zn^{2+} (Figure 6B and 6C). The hydroxamic acid hydroxyl group replaces the water molecule that binds to the zinc in the apo-HDL structure described above. The hydroxamic acid also hydrogen bonds with both charge relay system histidines (hydroxyl oxygen to His131 Ne2, 2.8 Å; and nitrogen to His132 Ne2, 2.8 Å), and the Tyr297 hydroxyl group (2.4 Å; Figure 6B and 6C).

The 5-carbon long branched alkene chain of TSA fits snugly in the narrow portion of the pocket making multiple van der Waals contacts with all of the hydrophobic groups lining the pocket (Figure 6B and 6C). Near its center, the chain contains a methyl substituted carbon-carbon double bond which is sandwiched between the phenyl groups of the Phe141 and Phe98 at the tightest point of the pocket (Figure 6A and 6B). The length of the alkene chain appears optimal for spanning the length of the pocket, and allowing contacts both at the bottom and at the entrance of the pocket, although, the cap group of Formula (I) may provide length to span the pocket allowing for a shorter alkene chain (aliphatic chain).

At the entrance of the pocket, one face of the planar structure formed by the dimethylamino-phenyl and adjacent carbonyl groups of TSA makes contacts at the rim of the pocket (Pro22, Tyr91, Phe141; Figure 6B and 6C). This

- 36 -

packing is facilitated by the roughly 110° angle in the overall structure of TSA at the junction of the aliphatic chain and the dimethylamino-phenyl group (occurring at the sp³ hybridized C8 carbon). Upon TSA binding, the side chain of Tyr91, which is mostly solvent exposed, changes conformation to make space for the dimethylamino-phenyl group. This is the only change near the active site observed upon TSA binding.

10 The hydroxamic acid group is a common motif in zinc metalloprotease inhibitors. See U.S. Patent No. 5,919,940 and 5,917,090; See also, Grams et al., 1995, *Biochemistry* 34:14012-14020; Lovejoy et al., 1999, *Nat. Struct. Biol.* 6:217-221; and Holmes & Matthews, 1981, *Biochemistry* 20:6912-6920. Like TSA, these inhibitors also coordinate the active site zinc in a bidentate fashion using their hydroxamate hydroxyl and carbonyl oxygens, replace the nucleophilic water molecule with their hydroxamate hydroxyl groups and form hydrogen bonds to the general base (Grams et al., 1995, *Biochemistry* 34:14012-14020; Lovejoy et al., 1999, *Nat. Struct. Biol.* 6:217-221; and Holmes & Matthews, 1981, *Biochemistry* 20:6912-6920).

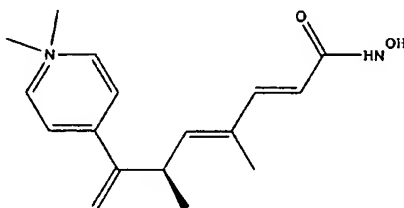
SAHA, which has a ~30-fold weaker inhibitory activity than TSA (Richon et al., 1998, *Proc. Natl. Acad. Sci. USA* 95:3003-3007), binds HDLP similarly to TSA (see, e.g., Figure 4D). The SAHA hydroxamic acid group makes the same contacts to the zinc and active site residues, and the importance of these interactions is underscored by the loss of activity of SAHA derivatives lacking the hydroxamic group (Richon et al., 1998, *Proc. Natl. Acad. Sci. USA* 95:3003-

- 37 -

3007). The six-carbon long aliphatic chain of SAHA packs in the tube-like hydrophobic portion of the pocket. Compared to TSA however, SAHA's aliphatic chain packs less snugly and makes fewer van der Waals contacts, in part, because SAHA lacks TSA's C15 methyl group branch. SAHA also lacks TSA's double bonds in this region, and this may lead to increased flexibility of the aliphatic chain. The cap group of SAHA consists of a phenyl-amino ketone group. In the crystal structure, the phenyl group has weak electron density, suggesting that it does not pack as well as the cap group of TSA. This may be due to the larger separation between the hydroxamic and cap groups of SAHA compared to TSA (compare TSA, Formula (II) and SAHA, Formula (III), below).

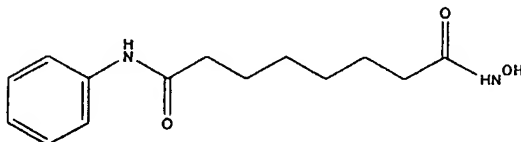
15 (II)

20



25 (III)

30



- 38 -

The determination of the structure of HDLP and HDLP bound to an inhibitory compound has enabled, for the first time, the identification of the active site of HDLP and of related HDLP proteins, such as proteins belonging to the HDAC family.

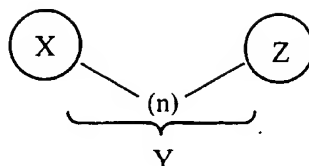
The three-dimensional structural information and the atomic coordinates associated with said structural information of HDLP bound to an inhibitory compound is useful in rational drug design providing for a method of identifying inhibitory compounds which bind to and inhibit the enzymatic activity of HDLP, HDAC family proteins and other histone deacetylase-like proteins related to HDLP. Said method for identifying said potential inhibitor for an enzyme comprising deacetylase activity comprises the steps of (a) using a three-dimensional structure of HDLP as defined by its atomic coordinates listed in Figure 16 to 19; (b) employing said three-dimensional structure to design or select said potential inhibitor; (c) synthesizing said potential inhibitor; (d) contacting said potential inhibitor with said enzyme in the presence of an acetylated substrate; and (e) determining the ability of said inhibitor to inhibit said deacetylase activity.

The potential HDLP and HDLP-related (e.g. HDAC) inhibitors identified by the method of the present invention are represented by formula (I)

30

- 39 -

(I)



5

wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of proline and leucine; Y comprises an aliphatic chain group which binds to
10 at least one amino acid selected from the group consisting of leucine, phenylalanine and glycine; and Z comprises an active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and wherein Z may further bind to a
15 zinc atom and with the provision that the compound of Formula (I) is not TSA, trapoxin, SAHA, SAHA derivatives described in U.S. Patent Nos. 5,608,108; 5,700,811; 5,773,474; 5840,960 and 5,668,179.

20 The present invention permits the use of molecular design techniques to design, identify and synthesize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site of HDLP and HDLP-related proteins. The atomic coordinates of apo-HDLP and
25 inhibitor-bound HDLP may be used in conjunction with computer modeling using a docking program such as GRAM, DOCK, HOOK or AUTODOCK (Dunbrack et al., 1997, *Folding & Design* 2:27-42) to identify potential inhibitors of HDLP and HDLP-related proteins (e.g. HDAC1). This procedure can
30 include computer fitting of potential inhibitors to the active site of HDLP to ascertain how well the shape and the

- 40 -

chemical structure of the potential inhibitor will complement the active site or to compare the potential inhibitors with the binding of TSA or SAHA in the active site. See Bugg et al, 1998, *Scientific American* 5 December:92-98; West et al., 1995, *TIPS* 16:67-74. The potential inhibitors designed by modeling with a docking program conform to the general formula (I) as described above. Computer programs may also be employed to estimate the attraction, repulsion and stearic hindrance of the HDLP 10 and potential inhibitor compound. Generally, the tighter the fit, the lower the stearic hindrances, the greater the attractive forces, and the greater the specificity which are important features for a specific inhibitory compound which is more likely to interact with HDLP and HDLP-related 15 proteins rather than other classes of proteins. These features are desired particularly where the inhibitory compound is a potential antitumor drug.

The compounds of the present invention may also be designed 20 by visually inspecting the three-dimensional structure to determine more effective deacetylase inhibitors. This type of modeling may be referred to as "manual" drug design. Manual drug design may employ visual inspection and analysis using a graphics visualization program such as "O" (Jones, 25 T.A., Zhou, J.Y., Cowan, S.W., and Kjeldgaard, M., Improved method for building protein models in electron density maps and the location of errors in these models, *Acta Crystallog.*, A47, 110-119.

30 Initially potential inhibitor compounds can be selected for their structural similarity to the X, Y and Z constituents

- 41 -

of formula (I) by manual drug design. The structural analog thus designed can then be modified by computer modeling programs to better define the most likely effective candidates. Reduction of the number of potential candidates is useful as it may not be possible to synthesize and screen a countless number of variations compounds that may have some similarity to known inhibitory molecules. Such analysis has been shown effective in the development of HIV protease inhibitors (Lam et al., 1994, *Science* 263:380-384; Wlodawer et al., 1993, *Ann. Rev. Biochem.* 62:543-585; Appelt, 1993 *Perspectives in Drug Discovery and Design* 1:23-48; Erickson, 1993, *Perspectives in Drug Discovery and Design* 1:109-128. Alternatively, random screening of an small molecule library could lead to potential inhibitors whose inhibitory activity may then be analyzed by computer modeling as described above to better determine their effectiveness as inhibitors.

The compounds designed using the information of the present invention may be competitive or noncompetitive inhibitors. These designed inhibitors may bind to all or a portion of the active site of HDLP and may be more potent, more specific, less toxic and more effective than known inhibitors for HDLP and HDLP-related proteins, and particularly HDACs. The designed inhibitors may also be less potent but have a longer half life in vivo and/or in vitro and therefore be more effective at inhibiting histone deacetylase activity in vivo and/or in vivo for prolonged periods of time. Said designed inhibitors are useful to inhibit the histone deacetylase activity of HDLP and HDLP-related proteins (e.g. HDAC1), to inhibit cell growth in

- 42 -

vitro and in vivo and may be particularly useful as antitumor agents.

5 The present invention also permits the use of molecular design techniques to computationally screen small molecule data bases for chemical entities or compounds that can bind to HDLP in a manner analogous to the TSA and SAHA as defined by the structure of the present invention. Such computational screening may identify various groups which
10 may be defined as "X", "Y" or "Z" of formula (I) above and may be employed to synthesize the potential inhibitors of the present invention comprising formula (I). Such potential inhibitors may be assayed for histone deacetylase inhibitory activity in a histone deacetylase activity assay
15 (see Example 3 below), may be co-crystallized with HDLP to determine the binding characteristics through X-ray crystallography techniques defined above (e.g. said co-crystal structure may be determined by molecular replacement to assess the binding characteristics of said potential
20 inhibitor), or may be assessed based on binding activity by incubating said potential inhibitor with said HDLP, performing gel filtration to separate any free potential inhibitor to HDLP-bound inhibitor, and determining the amount of histone deacetylase activity of the inhibitor-bound HDLP. To measure binding constants (e.g., Kd),
25 methods known to those in the art may be employed such as Biacore™ analysis, isothermal titration calorimetry, Elisa with a known drug on the plate to show competitive binding, or by a deacetylase activity assay.

The design of potential inhibitors of the present invention is further facilitated by reference to Figure 9, which is a surface representation figure that depicts the surface grooves. Analysis of such grooves gives insight into the constituents of the cap group of formula (I). The surface grooves are labeled groove A, groove A', groove B and groove C, into which additional cap groups may bind. The structure of HDLP bound to either TSA or SAHA shows that the cap groups of TSA and SAHA bind in groove A. By analysis of the amino acid sequence identity of HDLP and HDACs, Groove A is well conserved in HDACs, has a significant hydrophobic component, appears deep enough to allow for significant interactions and is also the largest of the four grooves. In addition to the dimethylamino phenyl group of the TSA, the A groove can fit approximately 200 daltons worth of groups (e.g. groove A could accommodate a naphthalene-like group after an appropriate spacer, etc.). Groove A, as referred to herein, is characterized by the following conserved residues of HDLP: His 21, Pro22, Lys24, Phe141, Leu265 and Phe335. The periphery of groove A comprises unconserved residues. Additionally, Groove A', as referred to herein, comprises primarily unconserved residues.

Groove B is immediately adjacent to the pocket. Of significance is that the bottom of groove B comprises the N-epsilon nitrogen of His170, which coordinates the zinc through its N-delta nitrogen. Significant binding energy may be achieved by contacting the Ne proton of His170 with a carboxylic acid or sulfate group. In addition, groove B may be large enough to fit a phenyl group, the face of which may comprise a partial negative charge which may pack over the N-epsilon proton of His170. The conserved residues of

- 44 -

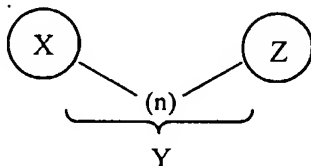
groove B, as referred to herein are: His170, Tyr196 and Leu265.

5 Groove C is not as well conserved as the other two grooves and the amino acid residues which comprise groove C are mostly polar and solvent exposed. Groove C, as referred to herein comprises the following conserved residues: Asn87, Gly140 and Phe198.

10 The compounds of the present invention are represented by formula (I):

(I)

15



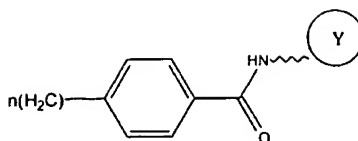
Examples for suitable X constituents wherein X comprises a cap group may be described in three categories, depending upon which surface of groove A, A', B and/or C they are targeted to. The cap group may comprise all three categories on the same compound. Of particular benefit may be replacing the cap group of TSA or SAHA with a large, rigid structure. Nonlimiting examples for suitable cap groups (X) of formula (I) which may bind in groove A are:

20 (1) attaching a 1-3 methyl linker followed by a phenyl or naphthalene group from the para or meta position of SAHA's phenyl group represented by formula (IV):

25

30

(IV)

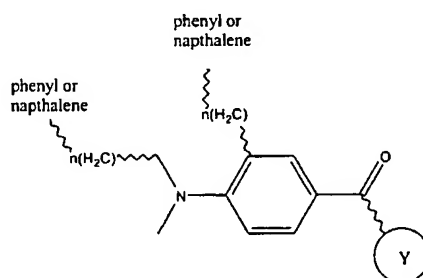


5

(2) attaching a 2-3 methyl linker followed by a phenyl or naphthalene group from the meta position of TSA's phenyl cap group, or from TSA's dimethyl amino group represented by formula (V):

10

(V)

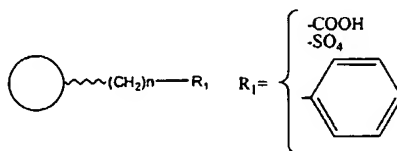


15

and which may bind in groove B is a 1-3 methyl group spacer followed by a carboxylate, sulfate or phenyl group as represented by formula (VI):

20

(VI)



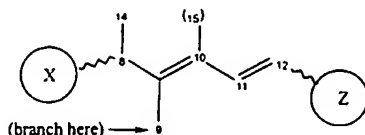
25

With respect to the aliphatic (Y) group, the diameter of the pocket suggests that one more methyl "side chain" could fit, in addition to the C15 methyl group on the C10 carbon. Nonlimiting suitable examples for Y constituents wherein Y comprises an aliphatic chain group are as follows: (1) add

30

a methyl group to TSA on the C12 carbon (with or without a methyl group on the C10 carbon and with or without double bonds and with or without substituting the X and/or Z constituents of formula (I) as represented by formula (VII):

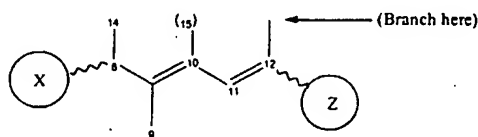
5 (VII)



10 (2) add a methyl group to TSA on the C9 carbon (with or without a methyl group on the C10 carbon; with or without both or either of the double bonds, and with or without substituting the X and/or Z constituents of formula (I) as represented by formula (VIII):

15

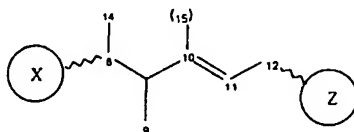
(VIII)



20

(3) replace the two alkalene double bonds of TSA with only one between C10 and C11, which may free the C11 and C12 torsion to allow for a better fit, the X and/or Z groups may also be substituted as represented by formula (IX):

25 (IX)

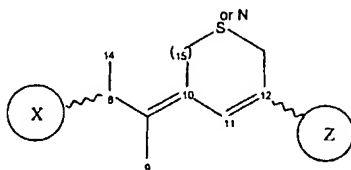


30

- 47 -

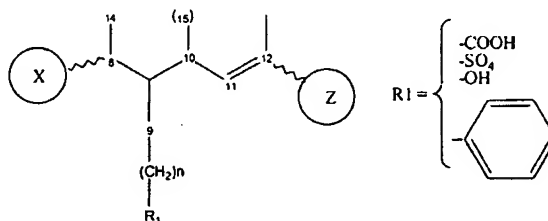
(4) cyclize C15 and C12 carbons of TSA through a sulphur atom (or nitrogen atom), the X and/or Z groups may also be substituted as represented by formula (X):

(X)



(5) extend from the C9 carbon of TSA such that the extension approaches and/or enters groove B (see Figure 9); making C9 sp³ so that it can have some freedom; attach to C9 a 1-3 methyl group spacer which may include a double bond and they attaching thereto a sulfate, carboxylate, sulfate, hydroxyl, or phenyl group which may make an interaction with the N-epsilon proton of His170 which may coordinate the zinc atom as represented by formula (XI):

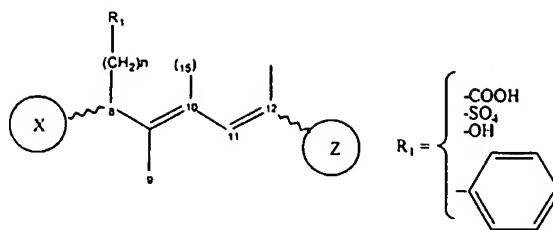
(XI)



(6) extend off the C8 carbon (replacing C14) of TSA such that the extension approaches or enters groove B; attach a 1-3 methyl group spacer (which may include a double bond) and then link thereto a carboxylate, sulfate, hydroxyl or phenyl group such that an interaction is made with the N-epsilon proton of His170 that coordinates the zinc atom; the X and/or Z constituents may also be substituted as represented by formula (XII):

(XII)

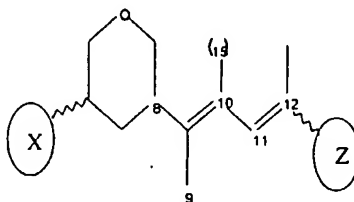
5



(7) substitute the C8 carbon at the end of the aliphatic chain such that the substitution may contact groove A, A', B and or C, in such an example, a cap group (X) may or may not be required and the X and Z constituents may be substituted as well, as represented by formula (XIII):

(XIII)

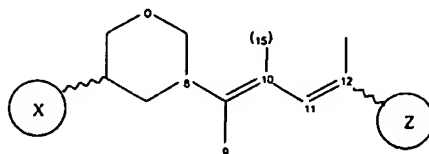
15



(8) formulas VII through XIII above wherein the aliphatic chain further comprises a methyl group between the active site binding group (Z) and the C8 carbon, and preferably just before the C8 carbon, increasing the distance between X and Z, (9) make the connection between the aliphatic chain and the cap group more rigid (e.g., by closing a 6-membered ring which may or may not comprise oxygen, the X and Z group may also be substituted as represented by formula (XIV):

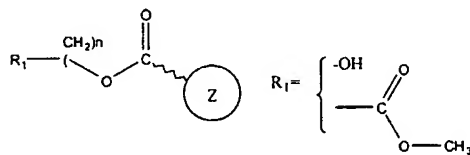
(XIV)

30

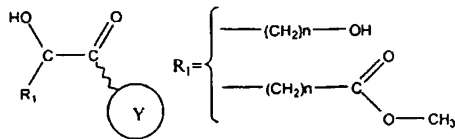


and (10) combining two or more of the changes depicted by formulas (VII-XIV).

Additionally, nonlimiting examples for suitable Z groups wherein Z comprises an active site binding group are as follows: (1) hydroxamic acid, (2) carboxylic acid, (3) sulfonamide, (4) acetamide, (5) epoxyketone, (6) an ester with a methyl linker and a hydroxyl of acetate ester group to lead into the cavity and interact with a conserved arginine (Arg27) as represented by formula (XV):
(XV)



and (7) an alphaketone as represented by formula (XVI):
(XVI)



Additionally, other suitable X, Y and Z constituents may be envisioned by the skilled artisan given the three-dimensional structural information of the present invention.

After having determined potential suitable X, Y and Z constituents, the constituents are combined to form a compound of formula (I) using combinatorial chemistry techniques. This may be achieved according to U.S. Patent Nos. 5,608,108; 5,700,811; 5,773,474; 5,840,960 and 5,668,179, incorporated herein by reference. Any methods

- 50 -

known to one of skill in the art may be employed to synthesize compounds of formula (I) comprising X, Y and Z constituents as determined by the methods described above.

5 As mentioned above, the compounds of formula (I) are useful to inhibit the histone deacetylase activity of HDLP and HDAC-related proteins. Such inhibition may allow for a reduction or cessation of cell growth *in vitro* and *in vivo*.

10 For *in vitro* use, such reduction or cessation of cell growth is useful to study the role of histone deacetylation and differentiation during the cell cycle and also to study other mechanisms associated with cell cycle arrest and particularly how the repression of transcription is involved
15 in cell cycle progression which may be studies in a yeast model system such as that described by Kadosh & Struhl, 1998, *Mol. Cell. Biol.* 18:5121-5127. *In vitro* model systems which may be employed to study the effects of potential inhibitors on cell cycle progression and also tumor growth
20 include those described by: Richon et al, 1998, *Proc. Natl. Acad. Sci. USA* 95:3003-3007; Yoshida et al., 1995, *Bioessays* 17:423-430; Kim et al., 1999, *Oncogene* 18:2461-2470; Richon et al., 1996, *Proc. Natl. Acad. Sci. USA* 93:5705-5708; and Yoshida et al., 1987, *Cancer Res.* 47:3688-3691.

25

For *in vivo* use, such a reduction or cessation of cell growth is useful to study the effect of said inhibitor compounds in non-human animal model systems of cancer and is also useful for the treatment of cancer in a recipient in
30 need of such treatment. Non-limiting examples of animals which may serve as non-human animal model systems include

- 51 -

mice, rats, rabbits, chickens, sheep, goats, cows, pigs, and non-human primates. See, e.g., Desai et al., 1999, *Proc. AACR* 40: abstract #2396; Cohen et al., 1999, *Cancer Res.*, submitted. The compounds of the present invention may be administered to a transgenic non-human animal wherein said animal has developed cancer such as those animal models in which the animal has a propensity for developing cancer (e.g. animal model systems described in U.S. Patents 5,777,193, 5,811,634, 5,709,844, 5,698,764, and 5,550,316). Such animal model systems may allow for the determination of toxicity and tumor reduction effectiveness of the compounds of the present invention.

A preferred compound of the present invention may comprise high specific activity for HDLP and HDAC-related proteins, good bioavailability when administered orally, activity in reducing or ceasing cell growth in tumor cell lines, and activity in reducing or ceasing tumor growth in animal models of various cancers.

Accordingly, another aspect of this invention is a method of eradicating or managing cancer in a recipient, which may be an animal and is preferably a human. Said method comprises administering to said recipient a tumor reducing amount of a compound as defined by formula (I) above, or a physiological acceptable salt thereof.

In a further aspect of the invention, there is provided a composition comprising the compound of formula (I) and an excipient or carrier. Administration of the foregoing agents may be local or systemic. Such carriers include any

- 52 -

suitable physiological solutions or dispersant or the like. The physiologic solutions include any acceptable solution or dispersion media, such as saline, or buffered saline. The carrier may also include antibacterial and antifungal agents, isotonic and absorption delaying agents, and the like. Except insofar as any conventional media, carrier or agent is incompatible with the active ingredient, its use in the compositions is contemplated.

Routes of administration for the compositions containing the delivery vehicle constructs of the present invention include any conventional and physiologically acceptable routes, such as, for example, oral, pulmonary, parenteral (intramuscular, intraperitoneal, intravenous (IV) or subcutaneous injection), inhalation (via a fine powder formulation or a fine mist), transdermal, nasal, vaginal, rectal, or sublingual routes of administration and can be formulated in dosage forms appropriate for each route of administration.

The following examples are provided to more clearly illustrate the aspects of the invention and are not intended to limit the scope of the invention.

EXAMPLES

Example 1: Protein Production and Purification:

Full-length wild-type HDLP (Genbank accession number AE000719) was subcloned from an *Aquifex aeolicus* chromosomal DNA preparation (provided by Robert Huber of Universitaet of Regensburg, Germany) into the pGEX4T3 (Amersham-Pharmacia, Piscataway, NJ) vector using the polymerase chain reaction (PCR). The cysteine-to-serine and active site mutants were constructed by PCR site directed mutagenesis and were

- 53 -

sequenced. The HDLP-glutathione S-transferase (GST) fusion protein was produced in *Escherichia coli*, purified by affinity chromatography using a column of glutathione-sepharose resin (Amersham-Pharmacia, Piscataway, NJ), and by anion-exchange chromatography (Q-sepharose™; Amersham-Pharmacia, Piscataway, NJ). HDLP was cleaved from the fusion protein with thrombin at 4° C, was purified by anion-exchange (Q-sepharose™; Amersham-Pharmacia, Piscataway, NJ) and gel filtration chromatography (Superdex™200; Amersham-Pharmacia, Piscataway, NJ), and was concentrated to typically 25 mg/ml in a buffer of 25 mM bis-tris propane (BTP), 500 mM NaCl, 5 mM dithiothrietirol (DTT), 2% isopropanol, pH 7.0.

Although, it is not known what metal cofactor HDLP contains *in vivo*, it is presumed to be zinc because of the arrangement of the ligands and the similarities in the active site to the zinc proteases. The lack of metal in the purified HDLP is presumed due, in part, to the use of DTT during purification. HDLP was reconstituted with Zn^{2+} by mixing the Cys75Ser/Cys77Ser double mutant at 10 mg/ml with a 5-fold molar excess of $ZnCl_2$ in a buffer of 25 mM bis-tris propane, 200 mM NaCl, 1% isopropanol, pH 7.0. Unbound $ZnCl_2$ was removed by fractionating HDLP through a G25 desalting column (Amersham-Pharmacia, Piscataway, NJ). The HDLP- Zn^{2+} -TSA complex was prepared by incubating the Zn^{2+} reconstituted HDLP mutant with 1 mM TSA for 45 minutes, followed by gel filtration chromatography (Superdex™200; Amersham-Pharmacia, Piscataway, NJ) to remove excess TSA, and concentration to typically 25 mg/ml in a buffer of 25 mM bis-tris propane, 500 mM NaCl, 1% isopropanol, pH 7.0.

- 54 -

FLAG epitope tagged human HDAC1 was overexpressed using a baculovirus expression system in Hi5 (Invitrogen, Carlsbad, CA) insect cells grown in suspension in serum-free media (Sf900, Gibco, Grand Island, NY). The fusion protein was purified by anion exchange and affinity chromatography using Anti-FLAG M2 affinity resin (Sigma, St. Louis, MO) and FLAG Peptide (Sigma,, St. Louis, MO).

Example 2: Crystallization and data collection:

Crystals of apo-HDLP were grown at room temperature by the hanging-drop vapor-diffusion method, from 7.5% isopropanol, 28% PEG 1500, 425 mM NaCl, 100 mM Tris-Cl, pH 7.0. They form in space group C2 with $a = 51.4 \text{ \AA}$, $b = 93.8 \text{ \AA}$, $c = 78.7 \text{ \AA}$, $\beta = 96.9 \text{ \AA}$, and contain one HDLP molecule in the asymmetric unit. Diffraction data were collected with crystals flash-frozen in a buffer of 7.5% isopropanol, 35% PEG 1500, 75 mM NaCl, 100 mM Tris-Cl, pH 8.0, at -170° C .

The structure of the HDLP- Zn^{2+} complex was determined from HDLP Cys75Ser/Cys77Ser double mutant crystals grown from 23% tert-butanol, 27% PEG 1500, 400 mM KCl, 100 mM bis-tris propane-Cl, pH 6.8. Space group and cell dimensions were identical to the apocrystals. The HDLP- Zn^{2+} crystals were harvested and frozen in 27% tert-butanol, 22% PEG 1500, 50 mM KCl, 20 mM NaCl, 0.2 mM ZnCl_2 , 100 mM bis-tris propane, pH 6.8, at -170° C .

Crystals of the HDLP- Zn^{2+} -TSA complex comprised HDLP Cys75Ser/Cys77Ser double mutant and were grown from 23% tert-butanol, 27% PEG 1500, 600 mM KCl, 100 mM bis-tris propane-Cl, pH 6.8, by microseeding. The crystals were grown in the presence of zinc. They form in space group

- 55 -

P2₁2₁2₁ with a = 53.4 Å, b = 94.4 Å, c = 156.3 Å and contain two HDLP- Zn²⁺-TSA complexes in the asymmetric unit. The HDLP-Zn²⁺-TSA crystals were harvested and frozen in the same cryobuffer as the HDLP- Zn²⁺ crystals except that 0.5mM TSA
5 was added. Data were processed with DENZO and SCALEPACK (Otwinowski & Minor, 1997, *Method. Ensemble.* 276:307-326). MIR analysis, model building and refinement.

The HDLP-Zn²⁺-SAHA complex crystals were grown and evaluated
10 the same as the HDLP-Zn²⁺-TSA crystals. However, the restraints for the SAHA structure were constructed based on stereochemical parameters from TSA. Like the apo-HDLP crystals, the SAHA/HDLP co-crystals grew in space group C2.

15 Heavy-atom soaks were performed with the apo-HDLP crystals in a buffer of 7.5% isopropanol, 30% PEG 1500, 75 mM NaCl, 100 mM Tris-Cl, pH 8.0, supplemented with 1.0 mM thimerosal for 2h, 5 mM KAu(CN)₂ for 1h, and 1 mM Pb(Me)₃OAc for 2h. MIR phases were calculated with the program MLPHARE (The
20 CCP4 suite: Programs for computational crystallography, 1994, *Acta Crystallogr. D* 50:760-763) at 2.5 Å using the anomalous diffraction signal from the thimerosal derivative, and had a mean figure of merit of 0.55. The phases were improved by solvent flattening with the program DM (The CCP4
25 suite: Programs for computational crystallography, 1994, *Acta Crystallogr. D* 50:760-763) , and were used to build the initial model with the program O (Jones et al., 1991, *Acta Crystallogr. A* 47:110-109). Successive rounds of rebuilding and simulated annealing refinement with the
30 program CNS (Brunger et al., 1998, *Acta Crystallogr. D* 54:905-921) allowed interpretation of HDLP from residues 2

- 56 -

to 373. Residues 1, 374, and 375 were not modeled and are presumed to be disordered.

The structure of the HDLP-Zn²⁺-TSA and HDLP-Zn²⁺-SAHA complex were determined by molecular replacement with the program AMORE (The CCP4 suite: Programs for computational crystallography, 1994, *Acta Crystallogr. D* 50:760-763) using the apo-HDLP structure as a search model. The initial electron density maps had strong and continuous difference density for the entire TSA molecule. However the SAHA molecule was not as well ordered in the cap group region. The structure of TSA was obtained from the Cambridge Structural Database (Refcode TRCHST) and was used to define stereochemical restraints used in the refinement with the program CNS. The restraints of SAHA were constructed based on stereochemical parameters from TSA and surrounding amino acid residues. The dimer interface in the HDLP-Zn²⁺-TSA and HDLP-Zn²⁺-SAHA crystals primarily involves Phe200 on the protein surface. The Phe200 side chain contacts Tyr91, whose side chain conformation changes on TSA binding, and part of the dimethyl amino phenyl group of TSA from the second protomer. The HDAC family does not contain a phenylalanine residue at the equivalent position.

25 Example 3: Histone deacetylase assays:

Purified proteins were assayed by incubating 10 µg of [³H]acetyl-labeled murine erythroleukemia histone substrate and HDAC assay buffer (20 mM Tris-HCl, pH 8.0, 150 mM NaCl, 10% glycerol) for 30-60 minutes at 37° C in a total volume of 30 µl. The final concentrations of HDLP and HDAC1-FLAG were 3.6 µM and 0.24 µM, respectively. Assays were performed in duplicate. The reactions were stopped and the

- 57 -

released acetate was extracted and assayed as described (Hendzel et al., 1991, *J. Biol. Chem.* 266:21936-21942). [3H]acetyl-labeled murine erythroleukemia histones were prepared essentially as described (Carmen et al., 1996, *J. Biol. Chem.* 271:15837-15844). Inhibitors were added in the
5 absence of substrate and incubated on ice for 20 minutes, substrate was added, and the assay performed as described above. HDLP was incubated with 20 μ M ZnCl_2 and 20 μ M $\text{MnCl}_2(\text{H}_2\text{O})_4$ in HDAC buffer and tested for activity.

10

Only HDLP dialyzed against ZnCl_2 had activity. HDAC1-FLAG was dialyzed against 20 μ M ZnCl_2 in HDAC buffer which had no effect on activity. Therefore, HDAC1-FLAG contains a metal as purified.

15

The *in vivo* substrate of HDLP is not known. HDLP may have a role in acetoin utilization like the *B. subtilis* AcuC gene product, and it has been annotated as such in the genome sequence, but the reaction catalyzed by AcuC is also not
20 known. Furthermore, the *A. aeolicus* genome appears to lack the acuA and acuB genes that are part of the acuABC operon of *B. subtilis* (Deckert et al., 1998 *Nature* 392:353-358), and HDLP is as similar to human HDAC1 (35.2 % identity) as it is to *B. subtilis* AcuC (34.7 % identity).

25

What is claimed is:

1. A crystal of an enzyme comprising deacetylase activity wherein said crystal effectively diffracts X-rays for the determination of the atomic coordinates of said enzyme to a resolution of greater than 4 Å and wherein the structure of said enzyme comprises a conserved core α/β structure characteristic fold wherein said conserved α/β fold comprises an eight-stranded parallel β sheet and eight α helices and wherein four of the helices pack on either face of said parallel β sheet and wherein said structure of said enzyme comprises an rmsd of less than or equal to 1.5 Å in the positions of C α atoms for at least 2/3 or more of the amino acids of HDLP as defined by the atomic coordinates of HDLP.
2. The crystal of claim 1, wherein said protein structure further comprises:
 - (a) eight α helices positioned near one side of the β sheet; and
 - (b) at least seven large, well defined loops originating from the C-terminal ends of the β -strands of said eight-stranded parallel β sheet wherein the eight extra helices and the seven large loops are associated with a significant extension of the structure beyond the core α/β motif and wherein said extension of the structure gives rise to a deep, narrow pocket and an internal cavity adjacent to the pocket.
3. The crystal of claim 1, wherein said enzyme comprising deacetylase activity is selected from the group

- 59 -

consisting of HDLP, HDLP-related proteins, HDAC1, HDAC2, HDAC3, HDAC4, HDAC5, HDAC6, HDAC-related proteins, APAH, AcuC, and functional derivatives thereof.

5

4. The crystal of claim 2 further comprising a specifically bound zinc atom in the active site of said enzyme.

10

5. The crystal of claim 2 further comprising a specifically bound deacetylase inhibitor compound in the active site of said enzyme.

15

6. The crystal of claim 2 define by the atomic coordinates according to Figure 16.

20

7. A method for identifying a potential deacetylase inhibitor compound for an enzyme which comprises deacetylase activity, said method comprising the steps of:

25

- a. using a three-dimensional structure of HDLP as defined by atomic coordinates according to Figure 16;
- b. employing said three-dimensional structure to design or select said potential inhibitor;
- c. synthesizing said potential inhibitor;
- d. contacting said potential inhibitor with said enzyme in the presence of an acetylated substrate; and
- e. determining the deacetylase inhibitory activity of said potential inhibitor.

30

- 60 -

8. The method of claim 7, wherein the three-dimensional structure is designed or selected using computer modeling.
- 5 9. The method of claim 7, wherein the potential deacetylase inhibitor is designed de novo.
10. The method of claim 7, wherein the potential deacetylase inhibitor is designed based on a known inhibitor.
10
11. The method of claim 7, wherein said enzyme comprising deacetylase activity is selected from the group consisting of HDLP, HDLP-related proteins, HDAC1, HDAC2, HDAC3, HDAC4, HDAC5, HDAC6, HDAC-related proteins, APAH, and AcuC.
15
12. A method of evaluating the binding properties of the potential deacetylase inhibitor compound comprising the steps of:
20
 - a. co-crystallizing said compound with HDLP;
 - b. determining the three-dimensional structure of said HDLP-potential inhibitor complex co-crystal by molecular replacement using the three-dimensional structure of HDLP as defined by atomic coordinates according to Figure 16; and
 - 25 c. analyzing said three-dimensional structure of said HDLP bound to said potential inhibitor compound to evaluate the binding characteristics of said potential inhibitor compound.
30
13. A method for solving the structure of an HDAC family

- 61 -

member crystal comprising the steps of:

- a. collecting X-ray diffraction data of said crystal wherein said data diffracts to a high resolution limit of greater than 4 Å;
 - 5 b. using the atomic coordinates of HDLP according to Figure 16 to perform molecular replacement or refinement and difference fourier with said X-ray diffraction data of said HDAC family member crystal to determine the structure of said HDAC family member; and
 - 10 c. refining said structure of said HDAC family member.
14. The method of claim 13, wherein said HDAC family member
15 is HDAC1.
 15. A Cys75Ser/Cys77Ser double mutant of HDLP wherein said mutant is encoded by the nucleic acid sequence of SEQ ID NO:4.
 - 20 16. A Cys75Ser/Cys77Ser double mutant of HDLP wherein said mutant has the amino acid sequence of SEQ ID NO:3.
 17. A nucleotide sequence according to SEQ ID NO:4
 - 25 18. An expression vector comprising the nucleotide sequence of claim 17.
 19. A method of using the crystal of claim 1 for screening
30 for a novel drug comprising:
 - a. selecting a potential ligand by performing

- 62 -

rational drug design with the three-dimensional structure determined for the crystal;

5 b. contacting the potential ligand with the ligand binding domain of the crystal; and

10 c. detecting the binding potential of the potential ligand for the ligand binding domain, wherein the novel drug is selected based on its having a greater affinity for the ligand binding domain than that of a known drug.

1/263

TABLE 1. Statistics from the crystallographic analysis

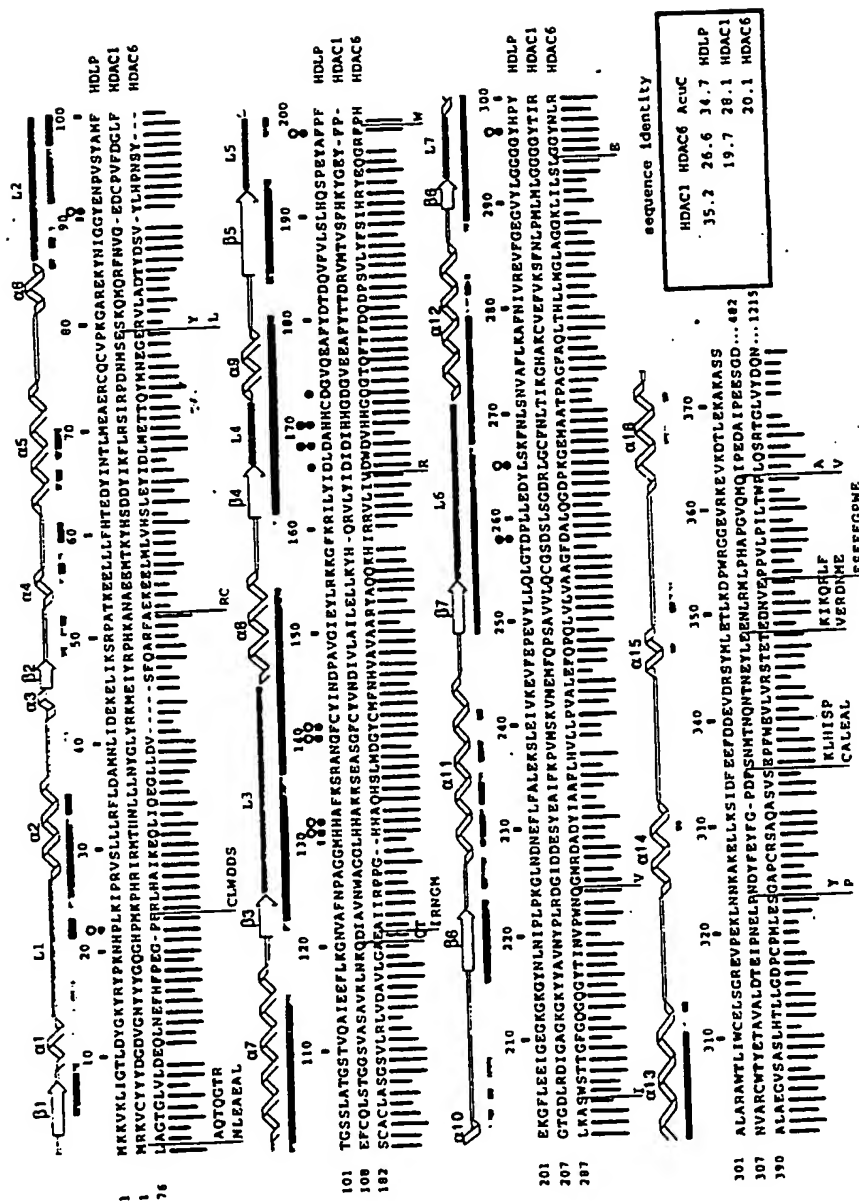
Data set	Native	thimerosal	Pb	AuCN	Zn	TSA			
Space Group	C2	C2	C2	C2	C2	P2 ₁ 2 ₁ 2 ₁			
Resolution (Å)	1.8	2.3	3.5	2.8	2.0	2.1			
Observations	134,952	79,023	11,454	27,722	125,769	180,427			
Unique reflections	32,143	15,958	4,040	8,753	23,643	50,796			
Data coverage (%)	92.3	95.7	86.4	94.3	90.6	93.8			
R _{sym} (%)	2.9	8.4	9.6	8.9	7.2	7.1			
MIR analysis (20.0-2.5 Å):									
phasing power	-	1.47	1.24	1.10	-	-			
R _{cullis}	-	0.72	0.78	0.85	-	-			
R _{cullis} (ano)		0.92							
Refinement statistics:						RMSD			
Data Set	Resolution (Å)	Reflections (I > 1σ)	Total atoms	Water atoms	R-factor (%)	R-free (%)	bonds (Å)	angles (°)	B-factor (Å ²)
HDLP	1.8	31,550	3214	228	19.8	24.0	0.010	1.63	3.55
HDLP-Zn	2.0	23,582	3424	434	22.0	25.8	0.009	1.48	1.04
HDLP-Zn-TSA	2.1	44,122	6475	456	22.4	25.8	0.008	1.78	3.83

$R_{\text{sym}} = \sum_h \sum_l |I_{h,l} - \langle I_h \rangle| / \sum_h \sum_l I_{h,l}$ for the intensity (I) of h observations of reflection h . Phasing power = $\langle F_A \rangle / E$, where $\langle F_A \rangle$ is the root-mean-square heavy atom structure factor and E is the residual lack of closure error.
 R_{cullis} is the mean residual lack of closure error divided by the dispersive difference. R -factor = $\sum |F_{\text{obs}} - F_{\text{calc}}| / \sum |F_{\text{obs}}|$, where F_{obs} and F_{calc} are the observed and calculated structure factors, respectively. Figure of merit = $|F(hkl)_{\text{best}}| / |F(hkl)|$. R -free = R -factor calculated using 5% of the reflection data chosen randomly and omitted from the start of refinement. RMSD: root mean square deviations from ideal geometry and root mean square variation in the B-factor of bonded atoms.

Figure 1

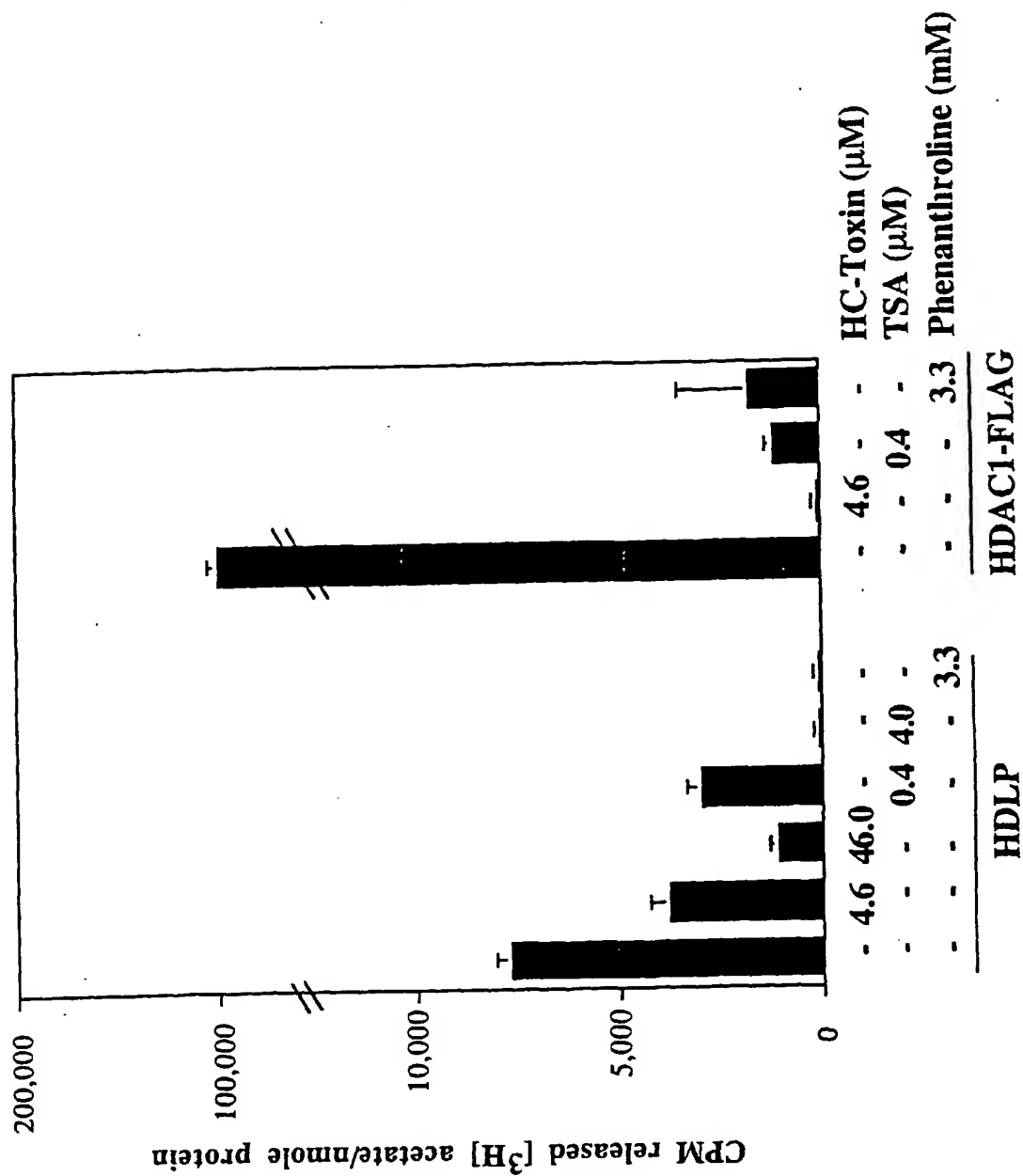
2/263

Figure 2



3/263

Figure 3



4/263

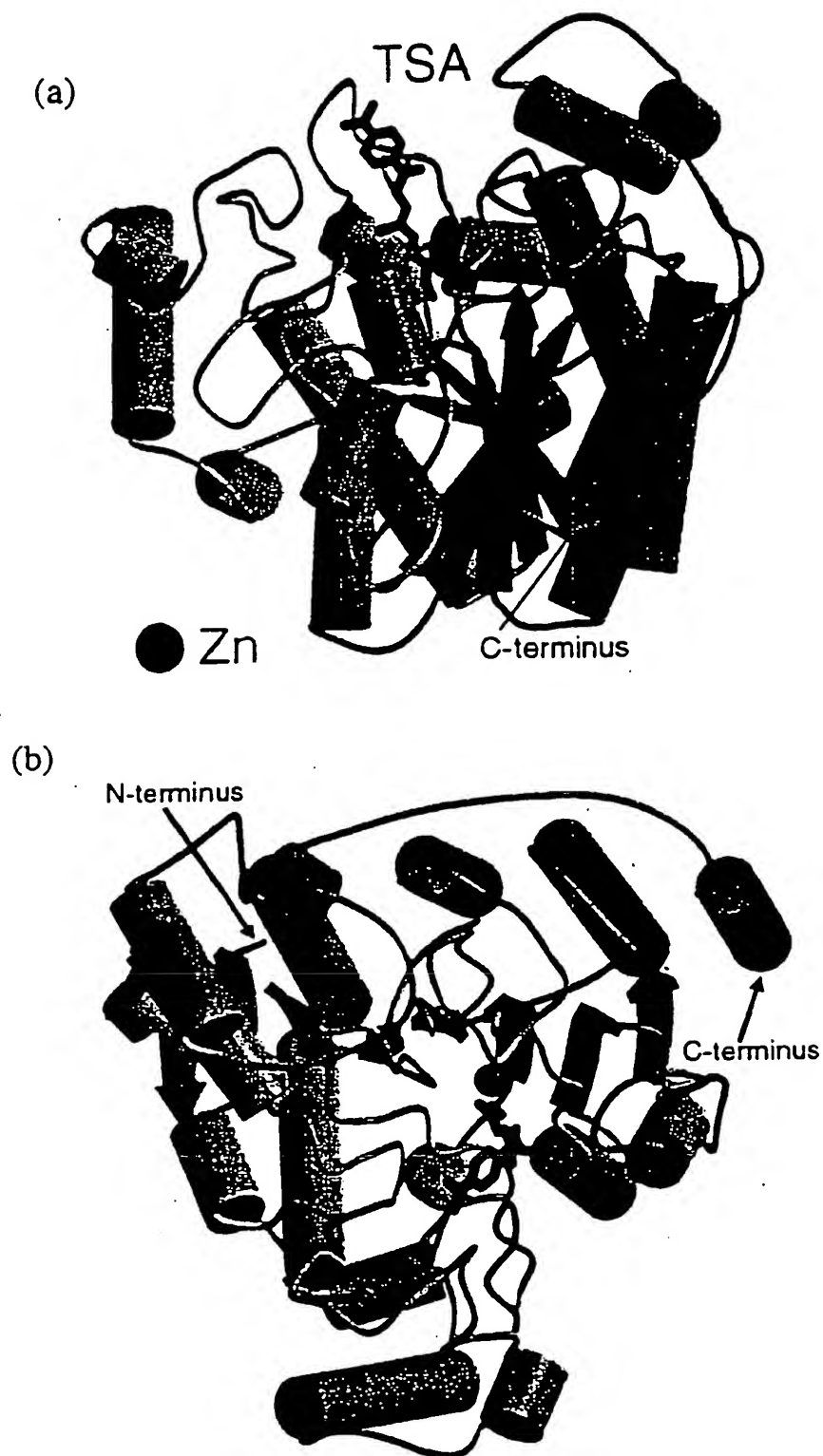
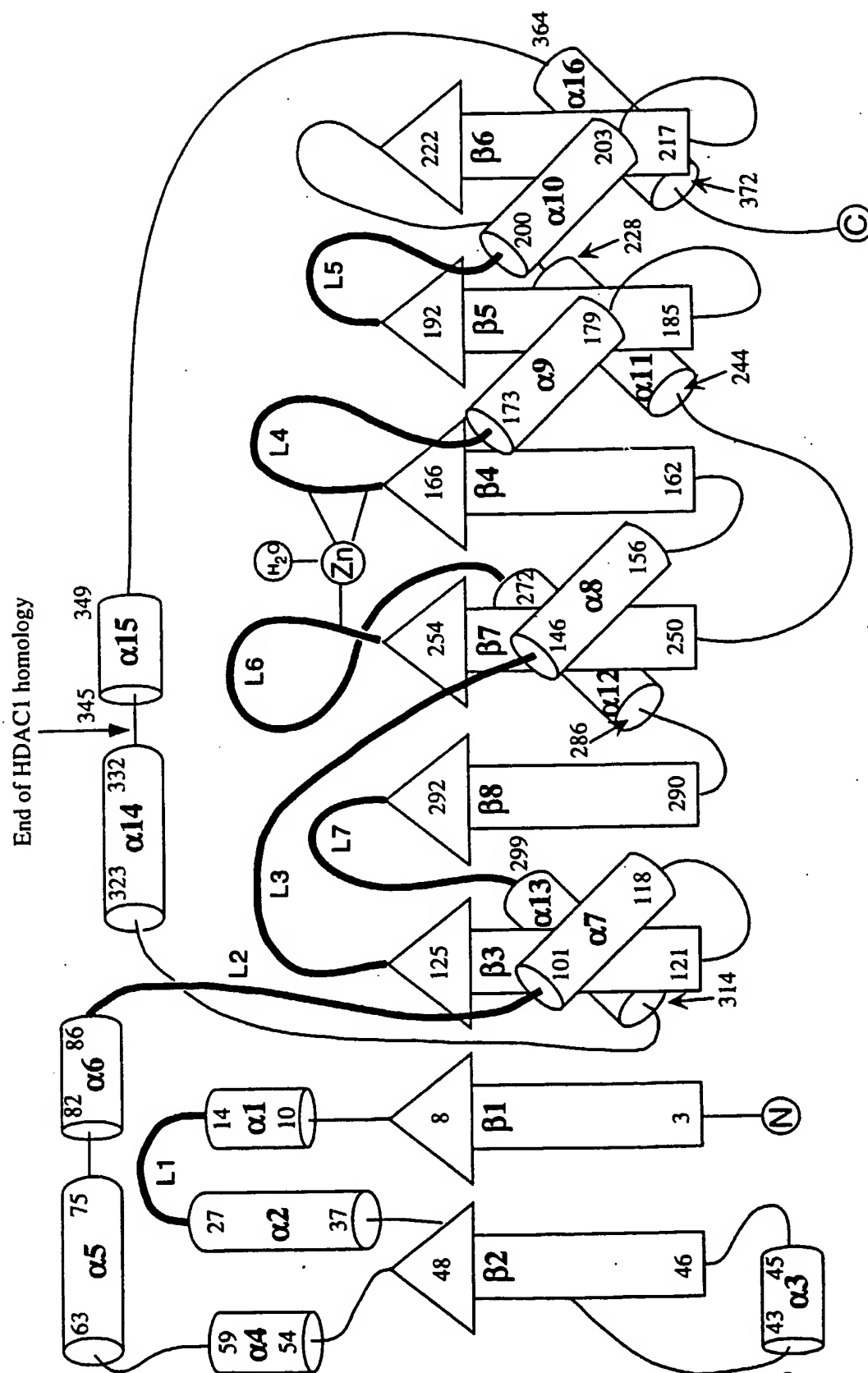


Figure 4

5/263

Figure 4C



6/263

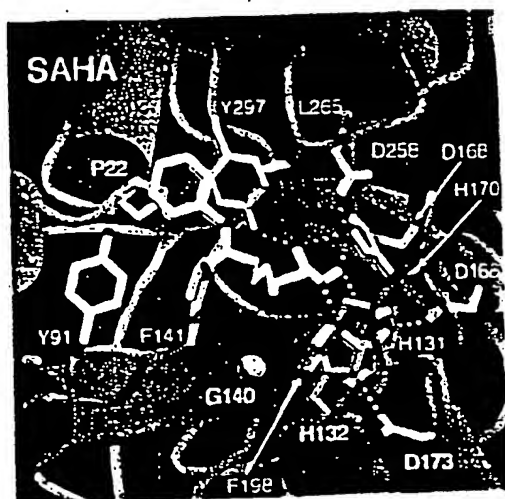
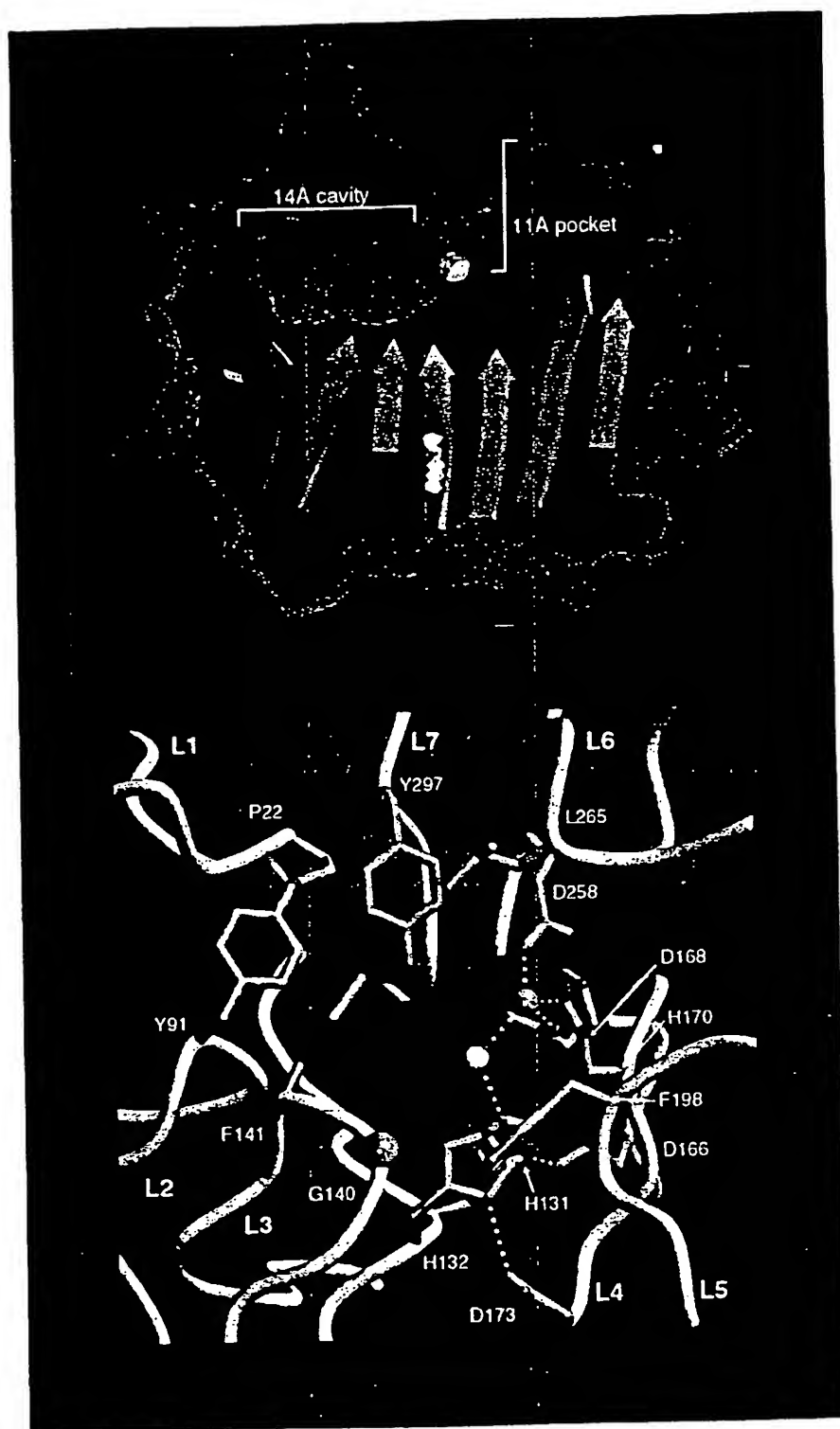


Figure 4D

Figure 5

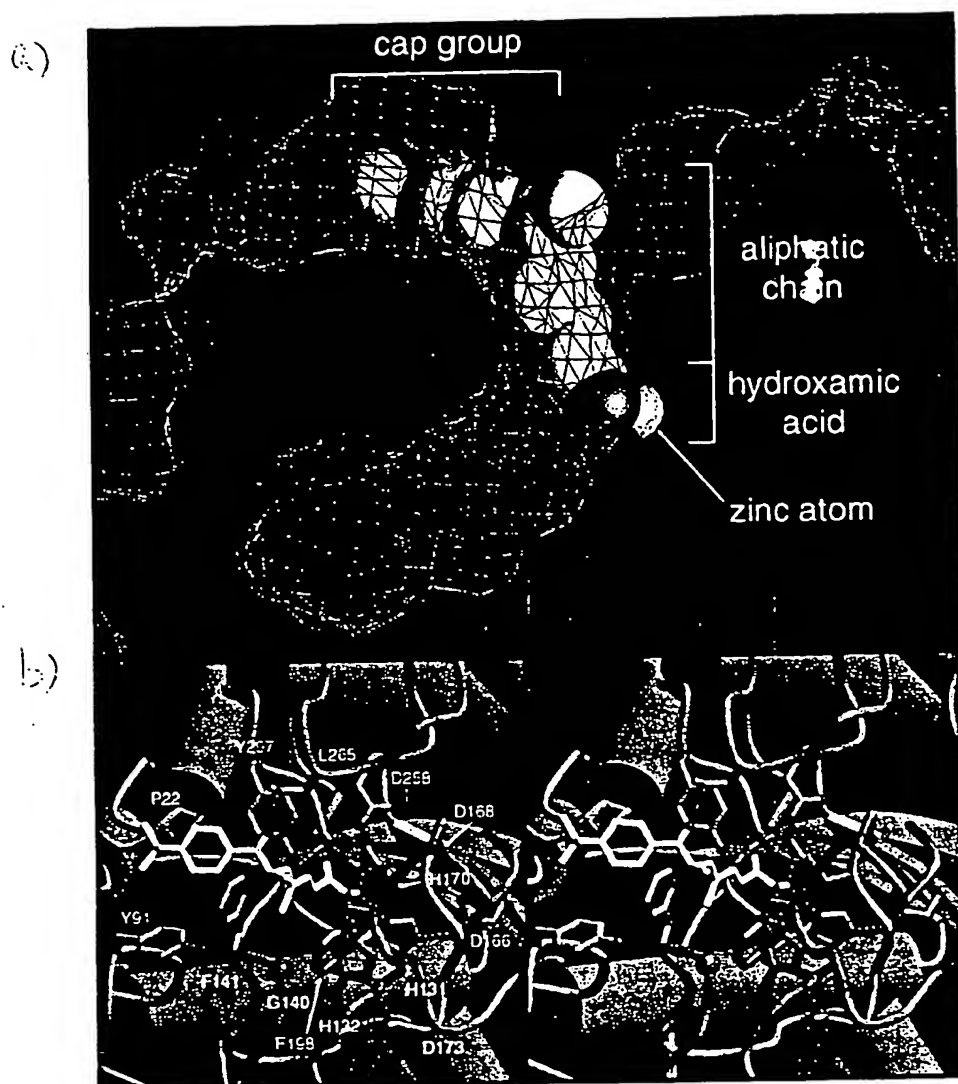
7/263

a)

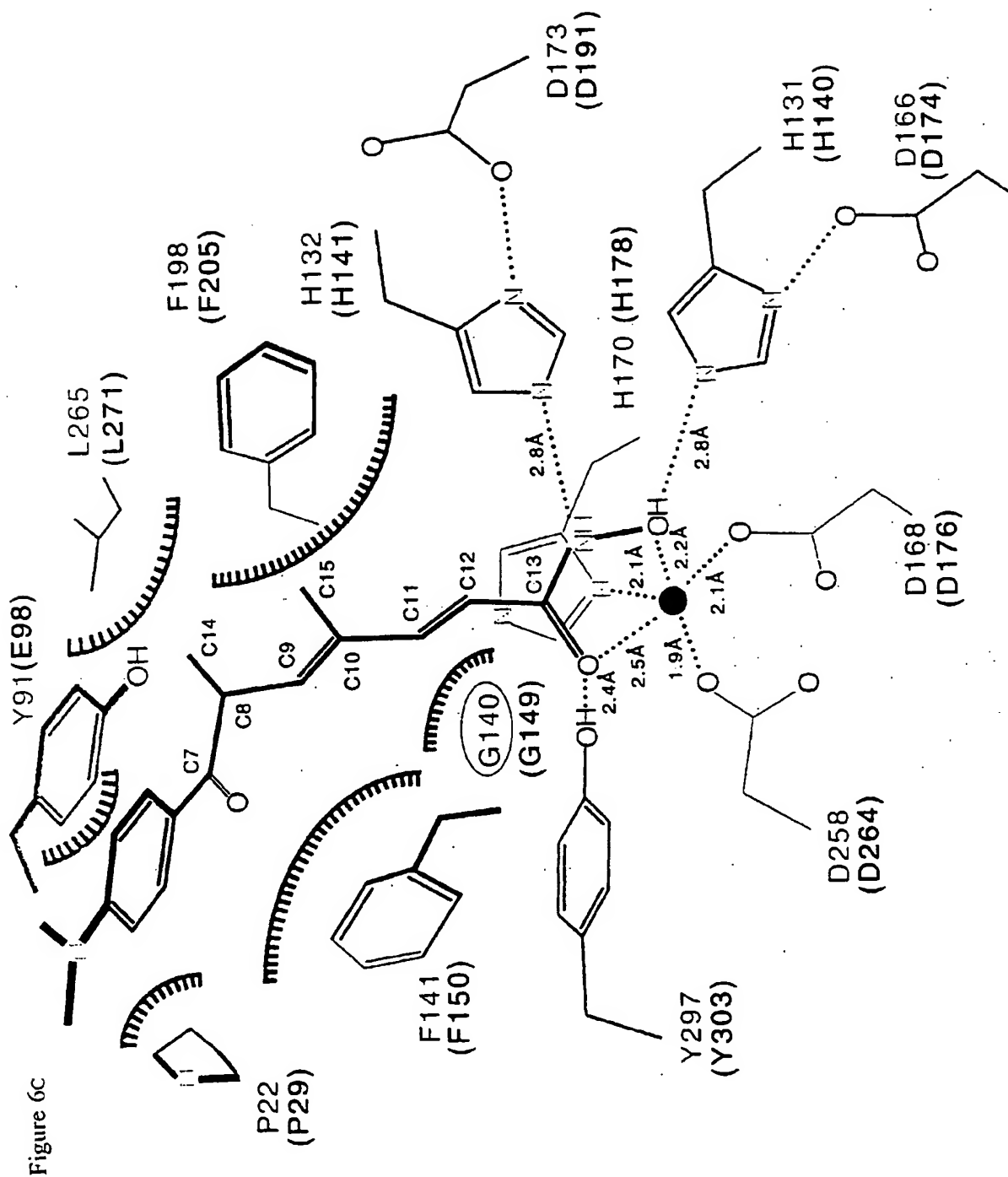


8/263

Figure 6



9/263




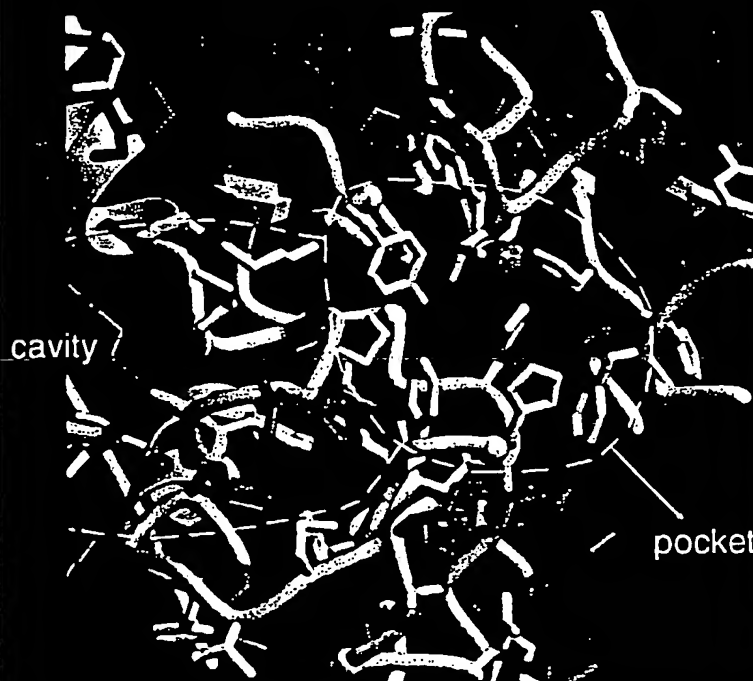

10/263

Figure 7

a)

 HDAC1 Identity

b)

 HDAC1 Identity  not conserved

11/263

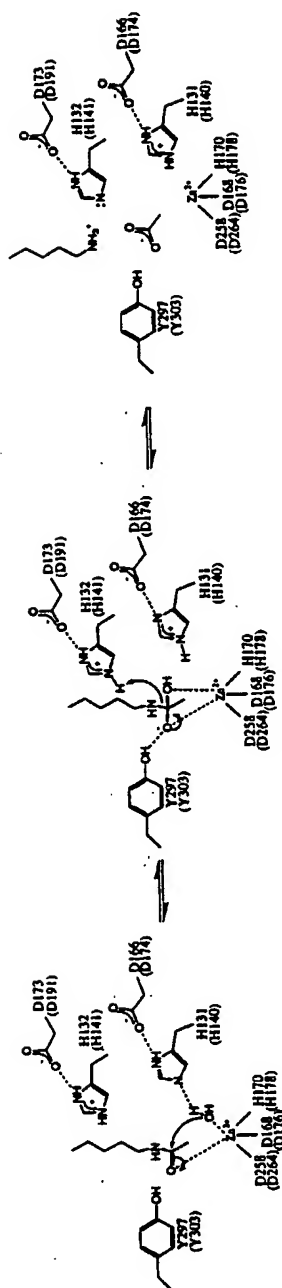


Figure 8

12/263

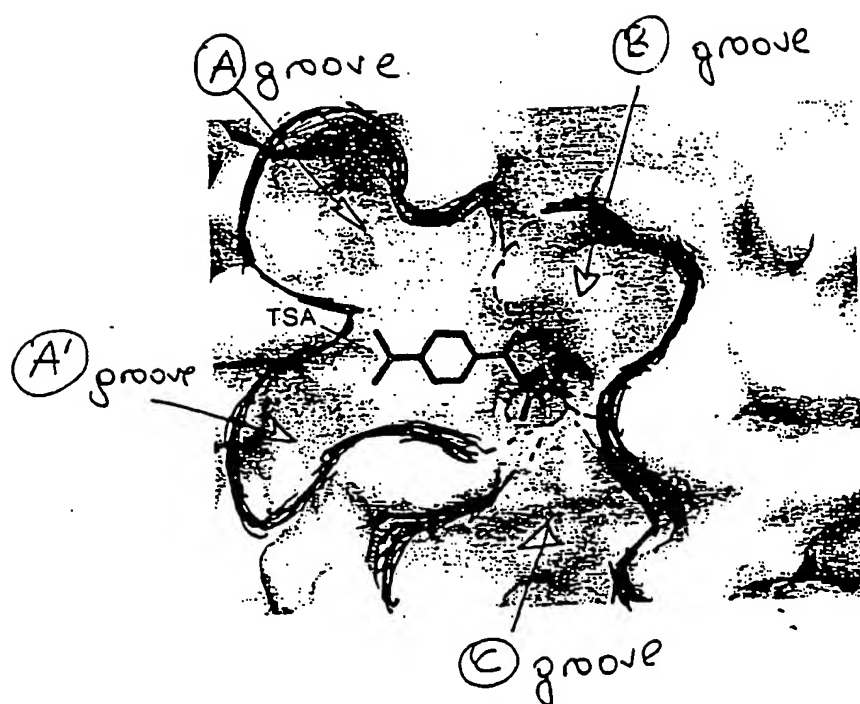


Figure 9

13/263

Figure 10

10 20 30 40
ATGAAGAAGGTTAAACTTATCGGAACCTTTAGACTACGGAA 40
AGTACAGATATCCCAAAAACCATCCTCTTAAAATACCAAG 80
AGTTTCCCTACTCCTTAGGTTTTTAGATGCCATGAACCTT 120
ATAGATGAGAAGGAATTAATCAAGAGCAGACCCGCAACTA 160
AAGAAGAACTCCTTTTATTCCACACGGAAGACTACATAAA 200

210 220 230 240
CACTTTAATGGAAGCGGAAAGGTGTCAGTCCGTTCCGAAG 240
GGAGCTAGGGAAAAGTACAACATAGGCGGATACGAAAACC 280
CCGTATCTTACGCGATGTTTACAGGCTCTTCTCTCGCAAC 320
GGGTTCAACAGTGCAGGCGATAGAGGAATTTTAAAGGGA 360
AATGTAGCTTTCAATCCCGCGGGAGGTATGCACCACGCTT 400

410 420 430 440
TTAAAAGCAGGGCAAACGGCTTTTGCTACATAAACGACCC 440
CGCTGTGGGAATTGAGTACTTGAGAAAAAAAGGCTTTAAG 480
AGAATACTCTACATAGACCTTGATGCCACCACCTGCGACG 520
GTGTTTCAGGAAGCCTTTTACGATACAGACCAGGTGTTTCGT 560
CCTGTCCCTTCACCAGTCGCCCCGAGTACGCCTTTCCCTTT 600

610 620 630 640
GAGAAGGGCTTCCTGGAGGAGATAGGAGAAGGAAAAGGAA 640
AGGGCTACAACCTGAACATTCCCCTGCCAAAGGGCTTGAA 680
CGACAACGAGTTCCCTCTTTGCCCTAGAAAAATCTCTGGAA 720
ATAGTCAAAGAAGTATTTGAGCCCGAGGTTTACCTTCTTC 760
AACTCGGAAGTGAACCACTCCTTGAAGATTACCTTTCCAA 800

810 820 830 840
GTTCAACCTCTCAAACGTTGCCTTTTTTAAAAGCTTTCAAC 840
ATCGTTTCGTGAGGTTTTTCGGGGAGGGAGTATACCTCGGAG 880
GAGGCGGATACCATCCTTACGCCCTCGCAAGGGCATGGAC 920
CCTAATCTGGTCCGAGCTTTTCGGGAAGGGAAGTCCCGGAA 960
AAGCTAAACAATAAAGCAAAAGAGCTTTTAAAGAGTATAG 1000

1010 1020 1030 1040
ACTTTGAAGAGTTTGAACGACGAGGTGGACCGCTCGTACAT 1040
GCTCGAAACCCTAAAGGACCCCTGGAGAGGAGGAGAGGTA 1080
AGGAAAGAAGTAAAGGATACGCTTGAAAAGCGAAAGCCT 1120
CATCTTA 1127

14/263

Figure 11

10 20 30 40
MKKVKLIGTLDYGKYRYPKNHPLKIPRVSLLLRFLDAMNL 40
IDKELIKSRPATKEELLLFHTEDYINTLMEAERCQCVPK 80
GAREKYNIGGYENPVSYAMFTGSSLATGSTVQAIEEFLKG 120
NVAFNPAAGMHAFKSRANGFCYINDPAVGIEYLKKKGFK 160
RILYIDLLDAHHCDCGVQEAIFYDTDQVFLSLHQSPFYAFPF 200
210 220 230 240
EKGFLLEETIGEGKGKGYNLNIPKGLNDNEFLFALEKSLE 240
IVKEVFEPEVYLLQLGTDPLLEDYLSKFNLNNVAFLKAFN 280
IVREVFGEVYLGGGGYHPYALARAWTLIWCELSGREVPE 320
KLNNKAKELLKSIDFEEFDDEVDRSYMLETCLKDEWRGGEV 360
RKEVKDTLEKAKASS 375

15/263

Figure 12

10 20 30 40
ATGAAGAAGGTTAACTTATCGGAAC TTAGACTACGGAA 40
AGTACAGATATCCCAAAAACCATCCTCTTAAAATACCAAG 80
AGTTTCCCTACTCCTTAGGTTTTTAGATGCCATGAACCTT 120
ATAGATGAGAAGGAATTAATCAAGAGCAGACCCGCAACTA 160
AAGAAGAACTCCTTTTATTCCACACGGAAGACTACATAAA 200
210 220 230 240
CACTTTTAATGGAAGCGGAAAGGTGT CAGTCCGTTCCGAAG 240
GGAGCTAGGGAAAAGTACAACATAGGCGGATACGAAAACC 280
CCGTATCTTACCGGATGTTTACAGGCTCTTCTCTCGCAAC 320
GGGTTC AACAGTGCAGGCGATAGAGGAATTTTTTAAAGGGA 360
AATGTAGCTTTCAATCCCGCGGGAGGTATGCACCACGCTT 400
410 420 430 440
TTAAAAGCAGGGCAAACGGCTTTTGCTACATAAAACGACCC 440
CGCTGTGGGAATTGAGTACTTGAGAAAAAAGGCTTTAAG 480
AGAATACTCTACATAGACCTTGATGCCCACTGCGACG 520
GTGTT CAGGAAGCCTTTTACGATACAGACCAGGTGTTCGT 560
CCTGTCCCTTCACCAGTCGCCCCGAGTACGCCTTTCCCTTT 600
610 620 630 640
GAGAAGGGCTTCCTGGAGGAGATAGGAGAAGGAAAAGGAA 640
AGGGCTACAACCTGAACATTCCCCTGCCAAAGGGCTTGAA 680
CGACAACGAGTTCCCTCTTTGCCCTAGAAAAATCTCTGGAA 720
ATAGTCAAAGAAGTATTTGAGCCCCGAGGTTTACCTTCTTC 760
AACTCGGAAC TGACCACTCCTTGAAGATTACCTTTCCAA 800
810 820 830 840
GTTCAACCTCTCAAACGTTGCCTTTTTTAAAAGCTTTCAAC 840
ATCGTTTCGTGAGGTTTTTCGGGGAGGGAGTATACCTCGGAG 880
GAGGCGGATTCCATCCTTACGCCCTCGCAAGGGCATGGAC 920
CCTAATCTGGTGCAGCTTTTCGGGAAGGGAAGTGCCGGAA 960
AAGCTAAACAATAAAGCAAAAGAGCTTTTTAAAGAGTATAG 1000
1010 1020 1030 1040
ACTTTGAAGAGTTTGACGACGAGGTGGACCGCTCGTACAT 1040
GCTCGAAACCCCTAAAGGACCCCTGGAGAGGAGGAGAGGTA 1080
AGGAAAGAAGTAAAGGATACGCTTGAAAAGGCGAAAGCCT 1120
CATCTA 1127

16/263

Figure 13

10 20 30 40
MKKVKLIGTLDYGKYRYPKNHPLKI PRVSLLLRFLDAMNL 40
IDKELIKSRPATKEELLLFHTEDYINTLMEAERCQCVPK 80
GAREKYNIGGYENPVSYAMFTGSSLATGSTVQAIEEFLKG 120
NVAFNPAGGMHHAFKSRANGFCYINDPAVGIEYLRKKGFK 160
RILYIDLDAHHC DG VQEAFYDIDQVFVLSLHQSP EYAFPF 200
210 220 230 240
EKGFL EEIGEGKGKGYNLNIPLPKGLNDNEFLFALEKSLE 240
IVKEVFEPEVYLLQLGTDPLLEDYLSKFNL SNVAF LKAFN 280
IVREVFGEGVYLG GGGFHPYALARA WTLIWCELSGREVPE 320
KLNNKAKELLKSIDFEEFDDEVDRSYMLET LKDPWRGGEV 360
RKEVKDTLEKAKASS 375

17/263

Figure 14

10 20 30 40
ATGAAGAAGGTTAACTTATCGGAACCTTAGACTACGGAA 40
AGTACAGATATCCCAAAACCATCCTCTTAAAATACCAAG 80
AGTTTCCCTACTCCTTAGGTTTTTAGATGCCATGAACCTT 120
ATAGATGAGAAGGAATTAATCAAGAGCAGACCCGCAACTA 160
AAGAAGAACTCCTTTTATTCCACACGGAAGACTACATAAA 200

210 220 230 240
CACTTTAATGGAAGCGGAAAGGAGTCAGAGCGTTCCGAAG 240
GGAGCTAGGGAAAAGTACAACATAGGCGGATACGAAAACC 280
CCGTATCTTACGCGATGTTTACAGGCTCTTCTCTCGCAAC 320
GGGTTCAACAGTGCAGGCGATAGAGGAATTTTAAAGGGA 360
AATGTAGCTTTCAATCCCGCGGGAGGTATGCACCACGCTT 400

410 420 430 440
TTAAAGCAGGGCAAACGGCTTTTGCTACATAAACGACCC 440
CGCTGTGGGAATTGAGTACTTGAGAAAAAAGGCTTTAAG 480
AGAATACTCTACATAGACCTTGATGCCCCACCACTGCGACG 520
GTGTTCAAGGAAGCCTTTTACGATACAGACCAGGTGTTTCGT 560
CCTGTCCCTTCACCAGTCGCCCCGAGTACGCCTTTCCCTTT 600

610 620 630 640
GAGAAGGGCTTCCTGGAGGAGATAGGAGAAGGAAAAGGAA 640
AGGGCTACAACCTGAACATTCCCCCTGCCAAAGGGCTTGAA 680
CGACAACGAGTTCTCTTTGCCCTAGAAAAATCTCTGGAA 720
ATAGTCAAAGAAGTATTTGAGCCCGAGGTTTACCTTCTTC 760
AACTCGGAACCTGACCCACTCCTTGAAGATTACCTTTCCAA 800

810 820 830 840
GTTCAACCTCTCAAACGTTGCCCTTTTAAAGCTTTCAAC 840
ATCGTTCTGTGAGGTTTTTCGGGGAGGGAGTATACCTCGGAG 880
GAGGCGGATACCATCCTTACGCCCTCGCAAGGGCATGGAC 920
CCTAATCTGGTGCGAGCTTTTCGGGAAGGGAAGTGCCGGAA 960
AAGCTAAACAATAAAGCAAAAGAGCTTTTAAAGAGTATAG 1000

1010 1020 1030 1040
ACTTTGAAGAGTTTGACGACGAGGTGGACCGCTCGTACAT 1040
GCTCGAAAACCTTAAAGGACCCCTGGAGAGGAGGAGAGGTA 1080
AGGAAAGAAGTAAAGGATACGCTTGAAAAGGCGAAAGCCT 1120
CATCTTA 1127

18/263

Figure 15

10 20 30 40
M K K V K L I G T L D Y G K Y R Y P K N H P L K I P R V S L L L R F L D A M N L 40
I D E K E L I K S R P A T K E E L L L F H T E D Y I N T L M E A E R S Q S V P K 80
G A R E K Y N I G G Y E N P V S Y A M F T G S S L A T G S T V Q A I E E F L K G 120
N V A F N P A G G M H A F K S R A N G F C Y I N D P A V G I E Y L R K K G F K 160
R I L Y I D L D A H H C D G V Q E A F Y D T D Q V F V L S L H Q S P E Y A F P F 200
210 220 230 240
E K G F L E E I G E G K G K G Y N L N I P L P K G L N D N E F L F A L E K S L E 240
I V K E V F E P E V Y L L Q L G T D P L L E D Y L S K F N L S N V A F L K A F N 280
I V R E V F G E G V Y L G G G G Y H P Y A L A R A W T L I W C E L S G R E V P E 320
K L N N K A K E L L K S I D F E E F D D E V D R S Y M L E T L K D P W R G G E V 360
R K E V K D T L E K A K A S S 375

19/263

Figure 16-1

				Residue #	X	Y	Z	OCC.	B	Segment ID
ATOM	1	CB	ALA	1	45.336	36.680	75.042	1.00	39.90	AAAA
ATOM	2	C	ALA	2	46.410	38.631	73.628	1.00	32.37	AAAA
ATOM	3	O	ALA	2	45.780	39.595	74.052	1.00	62.46	AAAA
ATOM	4	N	ALA	2	47.540	37.826	75.673	1.00	53.52	AAAA
ATOM	5	CA	ALA	2	46.668	37.432	74.527	1.00	57.32	AAAA
ATOM	6	N	LYS	3	46.390	38.570	73.389	1.00	39.61	AAAA
ATOM	7	CA	LYS	3	46.687	39.669	71.440	1.00	29.58	AAAA
ATOM	8	CB	LYS	3	47.355	39.763	70.459	1.00	36.03	AAAA
ATOM	9	CG	LYS	3	49.217	40.007	71.102	1.00	55.16	AAAA
ATOM	10	CD	LYS	3	50.313	40.000	70.039	1.00	65.28	AAAA
ATOM	11	CE	LYS	3	51.700	40.153	70.655	1.00	73.41	AAAA
ATOM	12	NZ	LYS	3	52.791	40.047	69.642	1.00	69.64	AAAA
ATOM	13	C	LYS	3	45.407	39.422	70.642	1.00	33.29	AAAA
ATOM	14	O	LYS	3	44.984	38.282	70.487	1.00	37.41	AAAA
ATOM	15	N	VAL	4	44.814	40.498	70.138	1.00	25.18	AAAA
ATOM	16	CA	VAL	4	43.385	40.418	69.349	1.00	22.30	AAAA
ATOM	17	CB	VAL	4	42.501	41.365	69.887	1.00	31.46	AAAA
ATOM	18	CG1	VAL	4	41.314	41.202	69.066	1.00	26.35	AAAA
ATOM	19	CG2	VAL	4	42.244	41.080	71.348	1.00	34.98	AAAA
ATOM	20	C	VAL	4	43.983	40.851	67.961	1.00	25.33	AAAA
ATOM	21	O	VAL	4	44.557	41.927	67.778	1.00	31.19	AAAA
ATOM	22	N	LYS	5	43.654	40.023	66.973	1.00	31.32	AAAA
ATOM	23	CA	LYS	5	44.052	40.291	65.607	1.00	20.20	AAAA
ATOM	24	CB	LYS	5	45.347	39.214	65.177	1.00	23.35	AAAA
ATOM	25	CG	LYS	5	46.301	39.092	65.049	1.00	23.75	AAAA
ATOM	26	CD	LYS	5	47.133	40.334	65.919	1.00	23.70	AAAA
ATOM	27	CE	LYS	5	48.510	40.151	65.669	1.00	24.34	AAAA
ATOM	28	NZ	LYS	5	49.151	41.357	65.585	1.00	22.04	AAAA
ATOM	29	C	LYS	5	42.314	40.294	64.596	1.00	20.27	AAAA
ATOM	30	O	LYS	5	41.949	39.535	64.728	1.00	18.48	AAAA
ATOM	31	N	LEU	6	43.071	41.111	63.564	1.00	19.28	AAAA
ATOM	32	CA	LEU	6	42.097	41.156	62.483	1.00	20.68	AAAA
ATOM	33	CB	LEU	6	41.571	42.574	62.291	1.00	23.51	AAAA
ATOM	34	CG	LEU	6	40.373	42.712	61.342	1.00	20.59	AAAA
ATOM	35	CD1	LEU	6	40.079	44.192	61.153	1.00	29.90	AAAA
ATOM	36	CD2	LEU	6	40.657	42.085	59.995	1.00	18.98	AAAA
ATOM	37	C	LEU	6	42.964	40.701	61.237	1.00	18.17	AAAA
ATOM	38	O	LEU	6	43.911	41.249	60.919	1.00	22.31	AAAA
ATOM	39	N	ILE	7	42.359	39.689	60.538	1.00	19.15	AAAA
ATOM	40	CA	ILE	7	43.045	39.199	59.338	1.00	18.38	AAAA
ATOM	41	CE	ILE	7	42.922	37.674	59.191	1.00	19.05	AAAA
ATOM	42	CG	ILE	7	43.920	37.162	58.144	1.00	16.45	AAAA
ATOM	43	CD1	ILE	7	43.353	37.007	60.551	1.00	22.81	AAAA
ATOM	44	CD2	ILE	7	43.086	35.543	60.450	1.00	14.99	AAAA
ATOM	45	C	ILE	7	42.396	39.650	58.115	1.00	17.95	AAAA
ATOM	46	O	ILE	7	41.188	39.729	57.928	1.00	19.07	AAAA
ATOM	47	N	GLY	8	43.193	40.562	57.330	1.00	17.70	AAAA
ATOM	48	CA	GLY	9	42.623	41.193	56.148	1.00	18.11	AAAA
ATOM	49	C	GLY	3	43.640	41.857	55.243	1.00	23.91	AAAA
ATOM	50	O	GLY	3	44.649	41.640	55.504	1.00	22.27	AAAA
ATOM	51	N	THR	9	43.134	42.428	54.155	1.00	23.99	AAAA
ATOM	52	CA	THR	9	43.950	43.141	53.183	1.00	25.25	AAAA
ATOM	53	CB	THR	9	44.739	42.195	52.263	1.00	25.30	AAAA
ATOM	54	CG1	THR	9	45.321	42.962	51.199	1.00	26.56	AAAA
ATOM	55	CG2	THR	9	43.823	41.144	51.557	1.00	25.24	AAAA
ATOM	56	C	THR	9	43.025	43.957	52.294	1.00	29.04	AAAA
ATOM	57	O	THR	9	41.872	43.582	52.082	1.00	23.05	AAAA
ATOM	58	N	LEU	10	43.517	45.079	51.781	1.00	29.19	AAAA
ATOM	59	CA	LEU	10	42.690	45.396	50.695	1.00	32.55	AAAA
ATOM	60	CB	LEU	10	43.056	47.319	50.761	1.00	28.09	AAAA
ATOM	61	CG	LEU	10	43.142	48.156	51.959	1.00	33.00	AAAA
ATOM	62	CD1	LEU	10	41.560	48.403	52.347	1.00	26.55	AAAA
ATOM	63	CD2	LEU	10	43.938	47.144	53.126	1.00	41.33	AAAA
ATOM	64	C	LEU	10	42.556	45.261	49.512	1.00	33.68	AAAA
ATOM	65	O	LEU	10	41.736	45.684	48.702	1.00	28.97	AAAA
ATOM	66	N	ASP	11	43.377	44.234	49.256	1.00	25.75	AAAA

20/263

Figure 16-2

ATOM	67	CA	ASP	11	43.367	43.541	47.970	1.00	35.74	AAAA
ATOM	68	CB	ASP	11	44.477	42.485	47.922	1.00	37.61	AAAA
ATOM	69	CG	ASP	11	45.858	43.093	48.079	1.00	46.75	AAAA
ATOM	70	OD1	ASP	11	46.110	44.136	47.444	1.00	46.34	AAAA
ATOM	71	OD2	ASP	11	46.690	42.528	48.821	1.00	58.94	AAAA
ATOM	72	C	ASP	11	42.034	42.898	47.607	1.00	34.26	AAAA
ATOM	73	O	ASP	11	41.748	42.696	46.420	1.00	31.12	AAAA
ATOM	74	N	TYR	12	41.220	42.558	48.609	1.00	26.19	AAAA
ATOM	75	CA	TYR	12	39.923	41.963	48.314	1.00	28.45	AAAA
ATOM	76	CB	TYR	12	39.119	41.720	49.601	1.00	29.35	AAAA
ATOM	77	CG	TYR	12	39.648	40.595	50.470	1.00	28.47	AAAA
ATOM	78	CD1	TYR	12	40.137	40.846	51.755	1.00	32.17	AAAA
ATOM	79	CE1	TYR	12	40.592	39.808	52.572	1.00	30.35	AAAA
ATOM	80	CD2	TYR	12	39.629	39.276	50.017	1.00	22.97	AAAA
ATOM	81	CE2	TYR	12	40.077	38.228	50.822	1.00	19.60	AAAA
ATOM	82	CZ	TYR	12	40.554	38.499	52.096	1.00	21.42	AAAA
ATOM	83	OH	TYR	12	40.964	37.456	52.907	1.00	23.49	AAAA
ATOM	84	C	TYR	12	39.144	42.907	47.390	1.00	26.67	AAAA
ATOM	85	O	TYR	12	38.307	42.466	46.593	1.00	30.51	AAAA
ATOM	86	N	GLY	13	39.441	44.201	47.492	1.00	30.22	AAAA
ATOM	87	CA	GLY	13	38.767	45.203	46.675	1.00	25.13	AAAA
ATOM	88	C	GLY	13	38.911	45.009	45.177	1.00	27.31	AAAA
ATOM	89	O	GLY	13	38.096	45.522	44.415	1.00	29.38	AAAA
ATOM	90	N	LYS	14	39.937	44.269	44.755	1.00	33.56	AAAA
ATOM	91	CA	LYS	14	40.176	44.005	43.337	1.00	39.81	AAAA
ATOM	92	CB	LYS	14	41.680	44.026	43.031	1.00	51.10	AAAA
ATOM	93	CG	LYS	14	42.292	45.424	42.907	1.00	64.99	AAAA
ATOM	94	CD	LYS	14	41.757	46.218	41.692	1.00	72.74	AAAA
ATOM	95	CE	LYS	14	42.183	45.639	40.336	1.00	67.25	AAAA
ATOM	96	NZ	LYS	14	41.637	44.280	40.045	1.00	70.06	AAAA
ATOM	97	C	LYS	14	39.589	42.688	42.834	1.00	39.98	AAAA
ATOM	98	O	LYS	14	39.746	42.350	41.658	1.00	46.99	AAAA
ATOM	99	N	TYR	15	38.927	41.944	43.717	1.00	32.64	AAAA
ATOM	100	CA	TYR	15	38.318	40.655	43.355	1.00	41.01	AAAA
ATOM	101	CB	TYR	15	38.996	39.512	44.126	1.00	26.48	AAAA
ATOM	102	CG	TYR	15	40.496	39.571	44.033	1.00	34.97	AAAA
ATOM	103	CD1	TYR	15	41.289	39.401	45.167	1.00	43.28	AAAA
ATOM	104	CE1	TYR	15	42.677	39.548	45.106	1.00	36.05	AAAA
ATOM	105	CD2	TYR	15	41.127	39.879	42.827	1.00	40.78	AAAA
ATOM	106	CE2	TYR	15	42.508	40.027	42.756	1.00	37.13	AAAA
ATOM	107	CZ	TYR	15	43.275	39.865	43.899	1.00	36.87	AAAA
ATOM	108	OH	TYR	15	44.644	40.044	43.844	1.00	35.40	AAAA
ATOM	109	C	TYR	15	36.838	40.705	43.714	1.00	38.62	AAAA
ATOM	110	O	TYR	15	36.344	39.868	44.468	1.00	37.82	AAAA
ATOM	111	N	ARG	16	36.141	41.703	43.177	1.00	44.85	AAAA
ATOM	112	CA	ARG	16	34.716	41.890	43.431	1.00	45.75	AAAA
ATOM	113	CB	ARG	16	34.320	43.348	43.187	1.00	54.17	AAAA
ATOM	114	CG	ARG	16	35.170	44.399	43.875	1.00	66.77	AAAA
ATOM	115	CD	ARG	16	34.920	44.506	45.369	1.00	72.39	AAAA
ATOM	116	NE	ARG	16	35.649	45.646	45.923	1.00	85.39	AAAA
ATOM	117	CZ	ARG	16	35.489	46.906	45.518	1.00	81.94	AAAA
ATOM	118	NH1	ARG	16	34.624	47.197	44.554	1.00	80.19	AAAA
ATOM	119	NH2	ARG	16	36.205	47.878	46.069	1.00	85.46	AAAA
ATOM	120	C	ARG	16	33.915	41.029	42.460	1.00	43.50	AAAA
ATOM	121	O	ARG	16	34.400	40.667	41.385	1.00	38.62	AAAA
ATOM	122	N	TYR	17	32.689	40.692	42.833	1.00	32.68	AAAA
ATOM	123	CA	TYR	17	31.850	39.923	41.930	1.00	37.55	AAAA
ATOM	124	CB	TYR	17	30.662	39.306	42.672	1.00	41.05	AAAA
ATOM	125	CG	TYR	17	31.040	38.104	43.519	1.00	37.51	AAAA
ATOM	126	CD1	TYR	17	32.039	38.194	44.493	1.00	32.59	AAAA
ATOM	127	CE1	TYR	17	32.383	37.095	45.277	1.00	29.32	AAAA
ATOM	128	CD2	TYR	17	30.393	36.875	43.346	1.00	31.46	AAAA
ATOM	129	CE2	TYR	17	30.726	35.772	44.122	1.00	28.64	AAAA
ATOM	130	CZ	TYR	17	31.721	35.887	45.088	1.00	27.14	AAAA
ATOM	131	OH	TYR	17	32.044	34.807	45.881	1.00	21.73	AAAA
ATOM	132	C	TYR	17	31.380	40.871	40.836	1.00	40.97	AAAA

21/263 Figure 16-3

ATOM	133	O	TYR	17	31.435	42.097	40.984	1.00	29.58	AAAA
ATOM	134	N	PRO	18	30.904	40.321	39.722	1.00	41.02	AAAA
ATOM	135	CD	PRO	18	30.760	38.910	39.318	1.00	48.67	AAAA
ATOM	136	CA	PRO	18	30.459	41.197	38.649	1.00	49.35	AAAA
ATOM	137	CB	PRO	18	30.321	40.228	37.481	1.00	59.04	AAAA
ATOM	138	CG	PRO	18	29.756	39.017	38.179	1.00	54.15	AAAA
ATOM	139	C	PRO	18	29.178	41.982	38.864	1.00	54.97	AAAA
ATOM	140	O	PRO	18	28.457	41.823	39.850	1.00	46.85	AAAA
ATOM	141	N	LYS	19	28.961	42.868	37.904	1.00	60.87	AAAA
ATOM	142	CA	LYS	19	27.777	43.696	37.749	1.00	67.78	AAAA
ATOM	143	CB	LYS	19	27.155	43.278	36.425	1.00	73.26	AAAA
ATOM	144	CG	LYS	19	26.971	41.752	36.414	1.00	77.87	AAAA
ATOM	145	CD	LYS	19	26.276	41.166	35.209	1.00	81.01	AAAA
ATOM	146	CE	LYS	19	26.039	39.680	35.471	1.00	82.45	AAAA
ATOM	147	NZ	LYS	19	25.417	38.959	34.331	1.00	83.11	AAAA
ATOM	148	C	LYS	19	26.688	43.594	38.814	1.00	64.15	AAAA
ATOM	149	O	LYS	19	26.810	44.047	39.949	1.00	65.73	AAAA
ATOM	150	N	ASN	20	25.604	42.986	38.345	1.00	59.78	AAAA
ATOM	151	CA	ASN	20	24.353	42.703	39.025	1.00	59.91	AAAA
ATOM	152	CB	ASN	20	23.516	41.844	38.077	1.00	68.08	AAAA
ATOM	153	CG	ASN	20	22.108	42.355	37.907	1.00	78.73	AAAA
ATOM	154	OD1	ASN	20	21.894	43.498	37.496	1.00	78.67	AAAA
ATOM	155	ND2	ASN	20	21.132	41.505	38.211	1.00	83.22	AAAA
ATOM	156	C	ASN	20	24.474	41.977	40.361	1.00	53.35	AAAA
ATOM	157	O	ASN	20	23.611	42.112	41.234	1.00	59.92	AAAA
ATOM	158	N	HIS	21	25.543	41.206	40.511	1.00	44.23	AAAA
ATOM	159	CA	HIS	21	25.768	40.397	41.707	1.00	28.15	AAAA
ATOM	160	CB	HIS	21	27.088	39.639	41.570	1.00	31.84	AAAA
ATOM	161	CG	HIS	21	27.155	38.411	42.418	1.00	34.79	AAAA
ATOM	162	CD2	HIS	21	27.344	38.259	43.752	1.00	25.03	AAAA
ATOM	163	ND1	HIS	21	26.929	37.148	41.917	1.00	34.81	AAAA
ATOM	164	CE1	HIS	21	26.979	36.269	42.900	1.00	17.01	AAAA
ATOM	165	NE2	HIS	21	27.228	36.917	44.026	1.00	32.31	AAAA
ATOM	166	C	HIS	21	25.763	41.135	43.051	1.00	29.37	AAAA
ATOM	167	O	HIS	21	26.346	42.210	43.186	1.00	28.54	AAAA
ATOM	168	N	PRO	22	25.093	40.565	44.066	1.00	29.14	AAAA
ATOM	169	CD	PRO	22	24.301	39.322	44.061	1.00	31.20	AAAA
ATOM	170	CA	PRO	22	25.034	41.185	45.395	1.00	32.84	AAAA
ATOM	171	CB	PRO	22	24.174	40.192	46.187	1.00	34.98	AAAA
ATOM	172	CG	PRO	22	23.257	39.634	45.109	1.00	30.11	AAAA
ATOM	173	C	PRO	22	26.411	41.415	46.044	1.00	34.37	AAAA
ATOM	174	O	PRO	22	26.554	42.272	46.916	1.00	29.17	AAAA
ATOM	175	N	LEU	23	27.415	40.644	45.629	1.00	29.22	AAAA
ATOM	176	CA	LEU	23	28.765	40.781	46.181	1.00	26.49	AAAA
ATOM	177	CB	LEU	23	29.414	39.397	46.332	1.00	22.30	AAAA
ATOM	178	CG	LEU	23	28.703	38.527	47.380	1.00	21.04	AAAA
ATOM	179	CD1	LEU	23	29.307	37.113	47.410	1.00	19.35	AAAA
ATOM	180	CD2	LEU	23	28.850	39.197	48.746	1.00	26.51	AAAA
ATOM	181	C	LEU	23	29.661	41.718	45.361	1.00	25.81	AAAA
ATOM	182	O	LEU	23	30.893	41.693	45.477	1.00	28.45	AAAA
ATOM	183	N	LYS	24	29.018	42.539	44.532	1.00	24.86	AAAA
ATOM	184	CA	LYS	24	29.696	43.552	43.723	1.00	27.35	AAAA
ATOM	185	CB	LYS	24	28.662	44.244	42.830	1.00	28.57	AAAA
ATOM	186	CG	LYS	24	29.118	45.532	42.171	1.00	52.95	AAAA
ATOM	187	CD	LYS	24	28.025	46.603	42.283	1.00	63.74	AAAA
ATOM	188	CE	LYS	24	26.688	46.138	41.706	1.00	66.09	AAAA
ATOM	189	NZ	LYS	24	25.595	47.137	41.896	1.00	66.00	AAAA
ATOM	190	C	LYS	24	30.332	44.592	44.676	1.00	29.52	AAAA
ATOM	191	O	LYS	24	31.412	45.123	44.420	1.00	30.67	AAAA
ATOM	192	N	ILE	25	29.652	44.879	45.779	1.00	26.90	AAAA
ATOM	193	CA	ILE	25	30.151	45.865	46.738	1.00	25.02	AAAA
ATOM	194	CB	ILE	25	29.105	46.177	47.824	1.00	28.34	AAAA
ATOM	195	CG2	ILE	25	27.961	46.951	47.237	1.00	23.84	AAAA
ATOM	196	CG1	ILE	25	28.661	44.869	48.495	1.00	30.31	AAAA
ATOM	197	CD1	ILE	25	27.718	45.051	49.660	1.00	44.90	AAAA
ATOM	198	C	ILE	25	31.424	45.463	47.483	1.00	32.19	AAAA

ATOM	199	O	ILE	25	31.736	44.271	47.623	1.00	26.54	AAAA
ATOM	200	N	PRO	26	32.191	46.463	47.956	1.00	30.14	AAAA
ATOM	201	CD	PRO	26	31.979	47.907	47.770	1.00	36.38	AAAA
ATOM	202	CA	PRO	26	33.431	46.241	48.707	1.00	30.63	AAAA
ATOM	203	CB	PRO	26	34.014	47.652	48.814	1.00	34.29	AAAA
ATOM	204	CG	PRO	26	33.397	48.373	47.617	1.00	43.39	AAAA
ATOM	205	C	PRO	26	32.943	45.727	50.061	1.00	25.99	AAAA
ATOM	206	O	PRO	26	31.854	46.110	50.484	1.00	25.51	AAAA
ATOM	207	N	ARG	27	33.719	44.880	50.743	1.00	21.98	AAAA
ATOM	208	CA	ARG	27	33.267	44.347	52.035	1.00	26.17	AAAA
ATOM	209	CB	ARG	27	32.641	42.969	51.834	1.00	22.70	AAAA
ATOM	210	CG	ARG	27	31.442	43.039	50.890	1.00	26.75	AAAA
ATOM	211	CD	ARG	27	30.832	41.672	50.581	1.00	33.22	AAAA
ATOM	212	NE	ARG	27	30.121	41.098	51.716	1.00	28.66	AAAA
ATOM	213	CZ	ARG	27	30.582	40.129	52.503	1.00	31.79	AAAA
ATOM	214	NH1	ARG	27	31.778	39.598	52.290	1.00	34.08	AAAA
ATOM	215	NH2	ARG	27	29.833	39.688	53.505	1.00	26.16	AAAA
ATOM	216	C	ARG	27	34.358	44.297	53.090	1.00	24.10	AAAA
ATOM	217	O	ARG	27	34.326	45.074	54.038	1.00	23.50	AAAA
ATOM	218	N	VAL	28	35.314	43.390	52.960	1.00	21.45	AAAA
ATOM	219	CA	VAL	28	36.385	43.385	53.953	1.00	21.75	AAAA
ATOM	220	CB	VAL	28	37.221	42.101	53.866	1.00	26.55	AAAA
ATOM	221	CG1	VAL	28	38.407	42.177	54.830	1.00	23.84	AAAA
ATOM	222	CG2	VAL	28	36.337	40.906	54.214	1.00	19.20	AAAA
ATOM	223	C	VAL	28	37.277	44.611	53.736	1.00	20.86	AAAA
ATOM	224	O	VAL	28	37.770	45.223	54.702	1.00	25.15	AAAA
ATOM	225	N	SER	29	37.480	44.996	52.475	1.00	19.22	AAAA
ATOM	226	CA	SER	29	38.320	46.169	52.209	1.00	19.63	AAAA
ATOM	227	CB	SER	29	38.591	46.352	50.702	1.00	24.45	AAAA
ATOM	228	OG	SER	29	37.411	46.697	49.984	1.00	28.74	AAAA
ATOM	229	C	SER	29	37.579	47.381	52.756	1.00	21.50	AAAA
ATOM	230	O	SER	29	38.184	48.320	53.271	1.00	18.95	AAAA
ATOM	231	N	LEU	30	36.256	47.353	52.673	1.00	19.56	AAAA
ATOM	232	CA	LEU	30	35.499	48.481	53.177	1.00	25.97	AAAA
ATOM	233	CB	LEU	30	34.032	48.396	52.744	1.00	22.90	AAAA
ATOM	234	CG	LEU	30	33.085	49.541	53.157	1.00	26.62	AAAA
ATOM	235	CD1	LEU	30	32.885	49.539	54.648	1.00	38.27	AAAA
ATOM	236	CD2	LEU	30	33.653	50.885	52.698	1.00	25.71	AAAA
ATOM	237	C	LEU	30	35.604	48.509	54.696	1.00	18.44	AAAA
ATOM	238	O	LEU	30	35.704	49.580	55.273	1.00	25.05	AAAA
ATOM	239	N	LEU	31	35.578	47.336	55.336	1.00	19.65	AAAA
ATOM	240	CA	LEU	31	35.672	47.270	56.797	1.00	20.47	AAAA
ATOM	241	CB	LEU	31	35.613	45.821	57.300	1.00	20.60	AAAA
ATOM	242	CG	LEU	31	34.988	45.456	58.665	1.00	39.80	AAAA
ATOM	243	CD1	LEU	31	35.712	44.219	59.257	1.00	23.99	AAAA
ATOM	244	CD2	LEU	31	35.085	46.591	59.637	1.00	28.48	AAAA
ATOM	245	C	LEU	31	37.009	47.870	57.229	1.00	23.85	AAAA
ATOM	246	O	LEU	31	37.070	48.673	58.154	1.00	21.24	AAAA
ATOM	247	N	LEU	32	38.079	47.462	56.562	1.00	23.91	AAAA
ATOM	248	CA	LEU	32	39.400	47.965	56.899	1.00	24.82	AAAA
ATOM	249	CB	LEU	32	40.479	47.320	56.018	1.00	24.81	AAAA
ATOM	250	CG	LEU	32	40.849	45.854	56.276	1.00	27.00	AAAA
ATOM	251	CD1	LEU	32	41.995	45.435	55.354	1.00	27.13	AAAA
ATOM	252	CD2	LEU	32	41.285	45.687	57.720	1.00	34.49	AAAA
ATOM	253	C	LEU	32	39.466	49.475	56.763	1.00	19.56	AAAA
ATOM	254	O	LEU	32	39.958	50.143	57.662	1.00	20.71	AAAA
ATOM	255	N	ARG	33	38.974	50.006	55.645	1.00	23.25	AAAA
ATOM	256	CA	ARG	33	39.007	51.449	55.441	1.00	24.33	AAAA
ATOM	257	CB	ARG	33	38.575	51.806	54.013	1.00	23.46	AAAA
ATOM	258	CG	ARG	33	39.571	51.327	52.945	1.00	26.94	AAAA
ATOM	259	CD	ARG	33	39.337	51.976	51.585	1.00	42.13	AAAA
ATOM	260	NE	ARG	33	38.023	51.661	51.037	1.00	59.06	AAAA
ATOM	261	CZ	ARG	33	37.583	52.088	49.857	1.00	60.87	AAAA
ATOM	262	NH1	ARG	33	38.353	52.850	49.095	1.00	65.33	AAAA
ATOM	263	NH2	ARG	33	36.373	51.743	49.433	1.00	56.24	AAAA
ATOM	264	C	ARG	33	38.124	52.156	56.455	1.00	30.33	AAAA

23/263

Figure 16-5

ATOM	265	O	ARG	33	38.441	53.252	56.905	1.00	25.45	AAAA
ATOM	266	N	PHE	34	37.022	51.514	56.828	1.00	24.98	AAAA
ATOM	267	CA	PHE	34	36.099	52.085	57.789	1.00	27.09	AAAA
ATOM	268	CB	PHE	34	34.798	51.276	57.807	1.00	24.88	AAAA
ATOM	269	CG	PHE	34	33.719	51.898	58.631	1.00	20.46	AAAA
ATOM	270	CD1	PHE	34	33.043	53.018	58.171	1.00	18.74	AAAA
ATOM	271	CD2	PHE	34	33.396	51.383	59.889	1.00	20.19	AAAA
ATOM	272	CE1	PHE	34	32.043	53.627	58.956	1.00	23.04	AAAA
ATOM	273	CE2	PHE	34	32.406	51.974	60.681	1.00	25.08	AAAA
ATOM	274	CZ	PHE	34	31.726	53.104	60.209	1.00	23.31	AAAA
ATOM	275	C	PHE	34	36.709	52.115	59.194	1.00	23.93	AAAA
ATOM	276	O	PHE	34	36.668	53.138	59.883	1.00	21.71	AAAA
ATOM	277	N	LYS	35	37.298	51.013	59.645	1.00	21.33	AAAA
ATOM	278	CA	LYS	35	37.862	51.084	60.978	1.00	22.54	AAAA
ATOM	279	CB	LYS	35	38.276	49.716	61.476	1.00	29.70	AAAA
ATOM	280	CG	LYS	35	37.082	48.890	61.924	1.00	29.48	AAAA
ATOM	281	CD	LYS	35	37.517	47.535	62.398	1.00	42.17	AAAA
ATOM	282	CE	LYS	35	38.157	46.762	61.275	1.00	34.89	AAAA
ATOM	283	NZ	LYS	35	39.372	47.412	60.719	1.00	67.18	AAAA
ATOM	284	C	LYS	35	39.027	52.055	61.040	1.00	24.68	AAAA
ATOM	285	O	LYS	35	39.282	52.640	62.085	1.00	22.33	AAAA
ATOM	286	N	ASP	36	39.724	52.231	59.926	1.00	25.67	AAAA
ATOM	287	CA	ASP	36	40.842	53.163	59.898	1.00	25.57	AAAA
ATOM	288	CB	ASP	36	41.669	52.984	58.621	1.00	32.26	AAAA
ATOM	289	CG	ASP	36	42.881	53.914	58.572	1.00	33.92	AAAA
ATOM	290	OD1	ASP	36	43.641	53.969	59.563	1.00	40.22	AAAA
ATOM	291	OD2	ASP	36	43.078	54.575	57.538	1.00	40.06	AAAA
ATOM	292	C	ASP	36	40.285	54.578	59.973	1.00	28.04	AAAA
ATOM	293	O	ASP	36	40.761	55.397	60.765	1.00	29.52	AAAA
ATOM	294	N	ALA	37	39.272	54.864	59.159	1.00	23.32	AAAA
ATOM	295	CA	ALA	37	38.651	56.192	59.163	1.00	28.22	AAAA
ATOM	296	CB	ALA	37	37.506	56.251	58.119	1.00	25.93	AAAA
ATOM	297	C	ALA	37	38.127	56.549	60.565	1.00	28.41	AAAA
ATOM	298	O	ALA	37	38.186	57.708	60.972	1.00	29.27	AAAA
ATOM	299	N	MET	38	37.639	55.547	61.300	1.00	24.76	AAAA
ATOM	300	CA	MET	38	37.103	55.727	62.669	1.00	25.45	AAAA
ATOM	301	CB	MET	38	36.077	54.625	62.982	1.00	25.19	AAAA
ATOM	302	CG	MET	38	34.816	54.660	62.148	1.00	22.32	AAAA
ATOM	303	SD	MET	38	33.733	55.983	62.702	1.00	29.90	AAAA
ATOM	304	CE	MET	38	33.402	55.417	64.376	1.00	26.51	AAAA
ATOM	305	C	MET	38	38.203	55.667	63.744	1.00	26.42	AAAA
ATOM	306	O	MET	38	37.924	55.818	64.947	1.00	23.77	AAAA
ATOM	307	N	ASN	39	39.437	55.434	63.300	1.00	26.21	AAAA
ATOM	308	CA	ASN	39	40.607	55.308	64.170	1.00	28.53	AAAA
ATOM	309	CB	ASN	39	40.926	56.643	64.855	1.00	33.95	AAAA
ATOM	310	CG	ASN	39	41.153	57.751	63.858	1.00	29.46	AAAA
ATOM	311	OD1	ASN	39	41.930	57.596	62.925	1.00	36.28	AAAA
ATOM	312	ND2	ASN	39	40.472	58.880	64.046	1.00	40.03	AAAA
ATOM	313	C	ASN	39	40.374	54.223	65.205	1.00	30.07	AAAA
ATOM	314	O	ASN	39	40.682	54.390	66.395	1.00	25.47	AAAA
ATOM	315	N	LEU	40	39.814	53.105	64.744	1.00	28.19	AAAA
ATOM	316	CA	LEU	40	39.527	51.984	65.633	1.00	25.50	AAAA
ATOM	317	CB	LEU	40	38.060	51.562	65.514	1.00	32.14	AAAA
ATOM	318	CG	LEU	40	37.044	52.585	66.036	1.00	30.47	AAAA
ATOM	319	CD1	LEU	40	35.637	52.027	65.894	1.00	29.07	AAAA
ATOM	320	CD2	LEU	40	37.325	52.889	67.491	1.00	23.80	AAAA
ATOM	321	C	LEU	40	40.433	50.771	65.415	1.00	26.99	AAAA
ATOM	322	O	LEU	40	40.157	49.683	65.915	1.00	25.41	AAAA
ATOM	323	N	ILE	41	41.528	50.970	64.691	1.00	28.33	AAAA
ATOM	324	CA	ILE	41	42.459	49.882	64.459	1.00	25.08	AAAA
ATOM	325	CB	ILE	41	42.010	49.020	63.243	1.00	25.01	AAAA
ATOM	326	CG2	ILE	41	42.061	49.824	61.961	1.00	22.74	AAAA
ATOM	327	CG1	ILE	41	42.917	47.802	63.128	1.00	31.01	AAAA
ATOM	328	CD1	ILE	41	42.895	46.951	64.341	1.00	42.18	AAAA
ATOM	329	C	ILE	41	43.900	50.376	64.247	1.00	24.09	AAAA
ATOM	330	O	ILE	41	44.128	51.406	63.621	1.00	28.92	AAAA

24/263

Figure 16-6

ATOM	331	N	ASP	42	44.866	49.634	64.787	1.00	28.95	AAAA
ATOM	332	CA	ASP	42	46.279	49.988	64.638	1.00	32.52	AAAA
ATOM	333	CB	ASP	42	46.951	50.094	66.007	1.00	34.24	AAAA
ATOM	334	CG	ASP	42	46.267	51.097	66.911	1.00	51.23	AAAA
ATOM	335	OD1	ASP	42	46.079	52.250	66.467	1.00	50.19	AAAA
ATOM	336	OD2	ASP	42	45.924	50.736	68.062	1.00	53.00	AAAA
ATOM	337	C	ASP	42	46.985	48.919	63.808	1.00	31.13	AAAA
ATOM	338	O	ASP	42	46.594	47.758	63.838	1.00	26.71	AAAA
ATOM	339	N	GLU	43	48.036	49.312	63.092	1.00	29.99	AAAA
ATOM	340	CA	GLU	43	48.793	48.392	62.240	1.00	31.34	AAAA
ATOM	341	CB	GLU	43	50.078	49.045	61.724	1.00	36.12	AAAA
ATOM	342	CG	GLU	43	49.886	50.118	60.676	1.00	52.72	AAAA
ATOM	343	CD	GLU	43	51.214	50.556	60.083	1.00	60.39	AAAA
ATOM	344	OE1	GLU	43	51.928	49.688	59.536	1.00	70.32	AAAA
ATOM	345	OE2	GLU	43	51.550	51.755	60.163	1.00	60.38	AAAA
ATOM	346	C	GLU	43	49.196	47.070	62.859	1.00	38.04	AAAA
ATOM	347	O	GLU	43	49.125	46.024	62.209	1.00	36.83	AAAA
ATOM	348	N	LYS	44	49.636	47.103	64.105	1.00	28.26	AAAA
ATOM	349	CA	LYS	44	50.084	45.879	64.740	1.00	32.71	AAAA
ATOM	350	CB	LYS	44	50.974	46.245	65.927	1.00	44.28	AAAA
ATOM	351	CG	LYS	44	52.211	47.007	65.418	1.00	59.37	AAAA
ATOM	352	CD	LYS	44	53.187	47.449	66.491	1.00	68.87	AAAA
ATOM	353	CE	LYS	44	54.373	48.167	65.849	1.00	67.21	AAAA
ATOM	354	NZ	LYS	44	55.361	48.648	66.850	1.00	74.00	AAAA
ATOM	355	C	LYS	44	48.982	44.889	65.115	1.00	26.75	AAAA
ATOM	356	O	LYS	44	49.265	43.792	65.586	1.00	27.37	AAAA
ATOM	357	N	GLU	45	47.731	45.278	64.881	1.00	29.20	AAAA
ATOM	358	CA	GLU	45	46.580	44.414	65.165	1.00	21.58	AAAA
ATOM	359	CB	GLU	45	45.387	45.243	65.676	1.00	18.24	AAAA
ATOM	360	CG	GLU	45	45.551	45.828	67.077	1.00	26.57	AAAA
ATOM	361	CD	GLU	45	44.418	46.772	67.453	1.00	23.12	AAAA
ATOM	362	OE1	GLU	45	44.224	47.783	66.746	1.00	21.64	AAAA
ATOM	363	OE2	GLU	45	43.725	46.509	68.454	1.00	26.48	AAAA
ATOM	364	C	GLU	45	46.163	43.710	63.870	1.00	26.31	AAAA
ATOM	365	O	GLU	45	45.400	42.739	63.889	1.00	22.32	AAAA
ATOM	366	N	LEU	46	46.674	44.204	62.748	1.00	20.15	AAAA
ATOM	367	CA	LEU	46	46.317	43.642	61.448	1.00	25.80	AAAA
ATOM	368	CB	LEU	46	46.137	44.774	60.433	1.00	27.25	AAAA
ATOM	369	CG	LEU	46	45.763	44.397	58.997	1.00	37.72	AAAA
ATOM	370	CD1	LEU	46	44.356	43.810	58.984	1.00	39.46	AAAA
ATOM	371	CD2	LEU	46	45.822	45.632	58.101	1.00	35.43	AAAA
ATOM	372	C	LEU	46	47.305	42.623	60.896	1.00	28.88	AAAA
ATOM	373	O	LEU	46	48.513	42.860	60.862	1.00	31.98	AAAA
ATOM	374	N	ILE	47	46.791	41.469	60.482	1.00	16.92	AAAA
ATOM	375	CA	ILE	47	47.638	40.448	59.872	1.00	20.98	AAAA
ATOM	376	CB	ILE	47	47.412	39.046	60.513	1.00	21.51	AAAA
ATOM	377	CG2	ILE	47	48.115	37.958	59.696	1.00	20.32	AAAA
ATOM	378	CG1	ILE	47	47.947	39.040	60.950	1.00	20.71	AAAA
ATOM	379	CD1	ILE	47	49.450	39.207	62.052	1.00	38.87	AAAA
ATOM	380	C	ILE	47	47.227	40.417	58.406	1.00	24.50	AAAA
ATOM	381	O	ILE	47	46.036	40.279	58.101	1.00	20.74	AAAA
ATOM	382	N	LYS	48	48.195	40.550	57.500	1.00	18.73	AAAA
ATOM	383	CA	LYS	48	47.883	40.543	56.072	1.00	15.55	AAAA
ATOM	384	CB	LYS	48	49.095	40.991	55.239	1.00	16.52	AAAA
ATOM	385	CG	LYS	48	48.836	41.011	53.738	1.00	23.25	AAAA
ATOM	386	CD	LYS	48	50.072	41.451	52.957	1.00	32.69	AAAA
ATOM	387	CE	LYS	48	49.796	41.496	51.462	1.00	26.00	AAAA
ATOM	388	NZ	LYS	48	48.704	42.449	51.114	1.00	46.33	AAAA
ATOM	389	C	LYS	48	47.473	39.140	55.629	1.00	14.43	AAAA
ATOM	390	O	LYS	48	48.177	38.174	55.887	1.00	16.83	AAAA
ATOM	391	N	SER	49	46.343	39.049	54.945	1.00	16.61	AAAA
ATOM	392	CA	SER	49	45.838	37.780	54.439	1.00	14.33	AAAA
ATOM	393	CB	SER	49	44.517	37.984	53.694	1.00	13.21	AAAA
ATOM	394	OG	SER	49	43.509	38.613	54.492	1.00	16.86	AAAA
ATOM	395	C	SER	49	46.810	37.131	53.459	1.00	24.11	AAAA
ATOM	396	O	SER	49	47.463	37.815	52.663	1.00	19.59	AAAA

25/263

Figure 16-7

ATOM	397	N	ARG	50	46.890	35.805	53.519	1.00	16.83	AAAA
ATOM	398	CA	ARG	50	47.724	35.037	52.610	1.00	23.88	AAAA
ATOM	399	CB	ARG	50	48.805	34.247	53.366	1.00	27.48	AAAA
ATOM	400	CG	ARG	50	48.284	33.036	54.177	1.00	22.99	AAAA
ATOM	401	CD	ARG	50	49.453	32.263	54.759	1.00	25.20	AAAA
ATOM	402	NE	ARG	50	49.073	31.197	55.684	1.00	15.88	AAAA
ATOM	403	CZ	ARG	50	48.411	30.093	55.368	1.00	14.34	AAAA
ATOM	404	NH1	ARG	50	48.023	29.863	54.117	1.00	15.78	AAAA
ATOM	405	NH2	ARG	50	48.150	29.197	56.312	1.00	16.78	AAAA
ATOM	406	C	ARG	50	46.821	34.023	51.905	1.00	20.20	AAAA
ATOM	407	O	ARG	50	45.763	33.650	52.414	1.00	18.63	AAAA
ATOM	408	N	PRO	51	47.203	33.596	50.699	1.00	15.63	AAAA
ATOM	409	CD	PRO	51	48.322	34.028	49.850	1.00	19.45	AAAA
ATOM	410	CA	PRO	51	46.387	32.606	49.994	1.00	14.35	AAAA
ATOM	411	CB	PRO	51	47.076	32.514	48.629	1.00	17.73	AAAA
ATOM	412	CG	PRO	51	47.707	33.890	48.475	1.00	17.62	AAAA
ATOM	413	C	PRO	51	46.452	31.256	50.708	1.00	15.73	AAAA
ATOM	414	O	PRO	51	47.460	30.942	51.350	1.00	18.67	AAAA
ATOM	415	N	ALA	52	45.377	30.470	50.618	1.00	11.47	AAAA
ATOM	416	CA	ALA	52	45.375	29.117	51.161	1.00	9.78	AAAA
ATOM	417	CB	ALA	52	43.967	28.529	51.112	1.00	12.19	AAAA
ATOM	418	C	ALA	52	46.301	28.342	50.209	1.00	17.19	AAAA
ATOM	419	O	ALA	52	46.307	28.609	49.006	1.00	16.46	AAAA
ATOM	420	N	THR	53	47.081	27.392	50.723	1.00	16.40	AAAA
ATOM	421	CA	THR	53	47.952	26.615	49.843	1.00	16.32	AAAA
ATOM	422	CB	THR	53	49.109	25.959	50.612	1.00	15.82	AAAA
ATOM	423	OG1	THR	53	48.582	25.016	51.559	1.00	16.25	AAAA
ATOM	424	CG2	THR	53	49.923	27.030	51.336	1.00	14.34	AAAA
ATOM	425	C	THR	53	47.104	25.520	49.215	1.00	14.06	AAAA
ATOM	426	O	THR	53	46.012	25.241	49.690	1.00	17.87	AAAA
ATOM	427	N	LYS	54	47.599	24.903	48.145	1.00	16.10	AAAA
ATOM	428	CA	LYS	54	46.848	23.832	47.492	1.00	19.00	AAAA
ATOM	429	CB	LYS	54	47.671	23.245	46.339	1.00	22.92	AAAA
ATOM	430	CG	LYS	54	46.955	22.172	45.539	1.00	32.99	AAAA
ATOM	431	CD	LYS	54	45.787	22.733	44.757	1.00	51.34	AAAA
ATOM	432	CE	LYS	54	46.244	23.565	43.561	1.00	64.17	AAAA
ATOM	433	NZ	LYS	54	46.898	22.733	42.505	1.00	63.45	AAAA
ATOM	434	C	LYS	54	46.554	22.738	48.520	1.00	22.48	AAAA
ATOM	435	O	LYS	54	45.463	22.158	48.555	1.00	19.97	AAAA
ATOM	436	N	GLU	55	47.536	22.465	49.364	1.00	25.65	AAAA
ATOM	437	CA	GLU	55	47.389	21.432	50.383	1.00	25.08	AAAA
ATOM	438	CB	GLU	55	48.718	21.241	51.116	1.00	25.40	AAAA
ATOM	439	CG	GLU	55	48.703	20.185	52.199	1.00	48.95	AAAA
ATOM	440	CD	GLU	55	50.106	19.821	52.673	1.00	64.21	AAAA
ATOM	441	OE1	GLU	55	50.220	19.033	53.640	1.00	62.38	AAAA
ATOM	442	OE2	GLU	55	51.093	20.311	52.073	1.00	58.22	AAAA
ATOM	443	C	GLU	55	46.273	21.773	51.362	1.00	18.91	AAAA
ATOM	444	O	GLU	55	45.489	20.908	51.723	1.00	17.43	AAAA
ATOM	445	N	GLU	56	46.196	23.029	51.786	1.00	16.80	AAAA
ATOM	446	CA	GLU	56	45.137	23.432	52.698	1.00	17.24	AAAA
ATOM	447	CB	GLU	56	45.399	24.855	53.204	1.00	16.15	AAAA
ATOM	448	CG	GLU	56	46.709	24.941	54.009	1.00	14.41	AAAA
ATOM	449	CD	GLU	56	47.087	26.354	54.358	1.00	20.17	AAAA
ATOM	450	OE1	GLU	56	46.713	27.252	53.567	1.00	17.12	AAAA
ATOM	451	OE2	GLU	56	47.773	26.564	55.394	1.00	18.23	AAAA
ATOM	452	C	GLU	56	43.781	23.313	52.000	1.00	15.95	AAAA
ATOM	453	O	GLU	56	42.799	22.869	52.599	1.00	17.82	AAAA
ATOM	454	N	LEU	57	43.722	23.691	50.725	1.00	17.53	AAAA
ATOM	455	CA	LEU	57	42.466	23.579	49.989	1.00	16.34	AAAA
ATOM	456	CB	LEU	57	42.591	24.177	48.586	1.00	13.86	AAAA
ATOM	457	CG	LEU	57	42.773	25.707	48.552	1.00	15.24	AAAA
ATOM	458	CD1	LEU	57	42.923	26.182	47.101	1.00	19.30	AAAA
ATOM	459	CD2	LEU	57	41.546	26.380	49.207	1.00	15.14	AAAA
ATOM	460	C	LEU	57	42.016	22.126	49.868	1.00	18.46	AAAA
ATOM	461	O	LEU	57	40.824	21.823	49.972	1.00	17.27	AAAA
ATOM	462	N	LEU	58	42.975	21.234	49.636	1.00	16.43	AAAA

26/263

Figure 16-8

ATOM	463	CA	LEU	58	42.662	19.822	49.475	1.00	15.18	AAAA
ATOM	464	CB	LEU	58	43.788	19.113	48.727	1.00	16.09	AAAA
ATOM	465	CG	LEU	58	44.029	19.682	47.321	1.00	21.72	AAAA
ATOM	466	CD1	LEU	58	45.221	18.982	46.680	1.00	31.92	AAAA
ATOM	467	CD2	LEU	58	42.786	19.549	46.469	1.00	34.38	AAAA
ATOM	468	C	LEU	58	42.339	19.116	50.787	1.00	21.19	AAAA
ATOM	469	O	LEU	58	42.067	17.914	50.795	1.00	20.40	AAAA
ATOM	470	N	LEU	59	42.377	19.849	51.896	1.00	13.50	AAAA
ATOM	471	CA	LEU	59	41.958	19.261	53.173	1.00	15.58	AAAA
ATOM	472	CB	LEU	59	42.182	20.236	54.339	1.00	18.98	AAAA
ATOM	473	CG	LEU	59	43.619	20.537	54.774	1.00	22.57	AAAA
ATOM	474	CD1	LEU	59	43.640	21.654	55.808	1.00	19.88	AAAA
ATOM	475	CD2	LEU	59	44.255	19.253	55.339	1.00	26.71	AAAA
ATOM	476	C	LEU	59	40.446	18.979	53.043	1.00	17.55	AAAA
ATOM	477	O	LEU	59	39.897	18.112	53.724	1.00	18.02	AAAA
ATOM	478	N	PHE	60	39.766	19.737	52.179	1.00	14.64	AAAA
ATOM	479	CA	PHE	60	38.338	19.536	51.970	1.00	18.17	AAAA
ATOM	480	CB	PHE	60	37.519	20.694	52.557	1.00	18.80	AAAA
ATOM	481	CG	PHE	60	36.028	20.564	52.316	1.00	15.94	AAAA
ATOM	482	CD1	PHE	60	35.320	19.476	52.817	1.00	19.98	AAAA
ATOM	483	CD2	PHE	60	35.339	21.524	51.576	1.00	18.09	AAAA
ATOM	484	CE1	PHE	60	33.947	19.338	52.587	1.00	18.72	AAAA
ATOM	485	CE2	PHE	60	33.964	21.399	51.338	1.00	19.19	AAAA
ATOM	486	CZ	PHE	60	33.268	20.295	51.850	1.00	18.43	AAAA
ATOM	487	C	PHE	60	37.916	19.337	50.510	1.00	16.45	AAAA
ATOM	488	O	PHE	60	37.227	18.371	50.179	1.00	19.18	AAAA
ATOM	489	N	HIS	61	38.308	20.257	49.638	1.00	18.26	AAAA
ATOM	490	CA	HIS	61	37.913	20.163	48.235	1.00	14.47	AAAA
ATOM	491	CB	HIS	61	38.004	21.545	47.582	1.00	17.15	AAAA
ATOM	492	CG	HIS	61	36.968	22.494	48.084	1.00	14.20	AAAA
ATOM	493	CD2	HIS	61	35.645	22.580	47.816	1.00	11.05	AAAA
ATOM	494	ND1	HIS	61	37.237	23.477	49.012	1.00	23.25	AAAA
ATOM	495	CE1	HIS	61	36.121	24.131	49.291	1.00	13.35	AAAA
ATOM	496	NE2	HIS	61	35.143	23.606	48.579	1.00	21.07	AAAA
ATOM	497	C	HIS	61	38.695	19.157	47.417	1.00	18.29	AAAA
ATOM	498	O	HIS	61	39.828	18.819	47.761	1.00	17.50	AAAA
ATOM	499	N	THR	62	38.071	18.658	46.346	1.00	15.39	AAAA
ATOM	500	CA	THR	62	38.741	17.686	45.473	1.00	19.02	AAAA
ATOM	501	CB	THR	62	37.734	16.767	44.756	1.00	19.61	AAAA
ATOM	502	OG1	THR	62	36.795	17.548	44.006	1.00	22.05	AAAA
ATOM	503	CG2	THR	62	36.995	15.925	45.767	1.00	28.99	AAAA
ATOM	504	C	THR	62	39.595	18.398	44.440	1.00	23.22	AAAA
ATOM	505	O	THR	62	39.311	19.532	44.044	1.00	17.47	AAAA
ATOM	506	N	GLU	63	40.657	17.732	44.009	1.00	18.94	AAAA
ATOM	507	CA	GLU	63	41.571	18.324	43.046	1.00	22.44	AAAA
ATOM	508	CB	GLU	63	42.736	17.384	42.750	1.00	28.31	AAAA
ATOM	509	CG	GLU	63	43.885	17.476	43.708	1.00	60.37	AAAA
ATOM	510	CD	GLU	63	45.154	16.893	43.115	1.00	55.08	AAAA
ATOM	511	OE1	GLU	63	45.603	17.407	42.065	1.00	66.44	AAAA
ATOM	512	OE2	GLU	63	45.697	15.927	43.694	1.00	71.72	AAAA
ATOM	513	C	GLU	63	40.983	18.764	41.730	1.00	18.63	AAAA
ATOM	514	O	GLU	63	41.340	19.827	41.228	1.00	18.37	AAAA
ATOM	515	N	ASP	64	40.108	17.943	41.153	1.00	19.77	AAAA
ATOM	516	CA	ASP	64	39.508	18.277	39.864	1.00	17.88	AAAA
ATOM	517	CB	ASP	64	38.584	17.159	39.372	1.00	20.43	AAAA
ATOM	518	CG	ASP	64	37.429	16.884	40.330	1.00	42.71	AAAA
ATOM	519	OD1	ASP	64	36.415	16.291	39.899	1.00	45.01	AAAA
ATOM	520	OD2	ASP	64	37.537	17.243	41.521	1.00	51.77	AAAA
ATOM	521	C	ASP	64	38.701	19.582	39.964	1.00	21.90	AAAA
ATOM	522	O	ASP	64	38.726	20.410	39.042	1.00	17.35	AAAA
ATOM	523	N	TYR	65	37.980	19.750	41.072	1.00	16.17	AAAA
ATOM	524	CA	TYR	65	37.178	20.957	41.292	1.00	15.62	AAAA
ATOM	525	CB	TYR	65	36.258	20.796	42.529	1.00	12.04	AAAA
ATOM	526	CG	TYR	65	35.501	22.065	42.886	1.00	12.23	AAAA
ATOM	527	CD1	TYR	65	34.699	22.718	41.940	1.00	14.73	AAAA
ATOM	528	CE1	TYR	65	34.028	23.910	42.253	1.00	18.23	AAAA

27/263 Figure 16-9

ATOM	529	CD2	TYR	65	35.609	22.631	44.163	1.00	13.67	AAAA
ATOM	530	CE2	TYR	65	34.943	23.824	44.486	1.00	18.16	AAAA
ATOM	531	CZ	TYR	65	34.162	24.461	43.533	1.00	16.88	AAAA
ATOM	532	OH	TYR	65	33.555	25.665	43.837	1.00	14.59	AAAA
ATOM	533	C	TYR	65	38.090	22.177	41.459	1.00	15.27	AAAA
ATOM	534	O	TYR	65	37.882	23.189	40.798	1.00	15.96	AAAA
ATOM	535	N	ILE	66	39.098	22.073	42.321	1.00	14.29	AAAA
ATOM	536	CA	ILE	66	40.022	23.179	42.540	1.00	18.86	AAAA
ATOM	537	CB	ILE	66	41.090	22.836	43.617	1.00	15.56	AAAA
ATOM	538	CG2	ILE	66	42.152	23.943	43.698	1.00	20.45	AAAA
ATOM	539	CG1	ILE	66	40.405	22.659	44.967	1.00	19.68	AAAA
ATOM	540	CD1	ILE	66	39.717	23.948	45.454	1.00	29.11	AAAA
ATOM	541	C	ILE	66	40.716	23.519	41.236	1.00	25.20	AAAA
ATOM	542	O	ILE	66	40.809	24.692	40.895	1.00	14.60	AAAA
ATOM	543	N	ASN	67	41.190	22.508	40.498	1.00	18.21	AAAA
ATOM	544	CA	ASN	67	41.879	22.789	39.236	1.00	20.03	AAAA
ATOM	545	CB	ASN	67	42.448	21.523	38.580	1.00	21.73	AAAA
ATOM	546	CG	ASN	67	43.645	20.954	39.333	1.00	21.69	AAAA
ATOM	547	OD1	ASN	67	44.293	21.645	40.110	1.00	23.97	AAAA
ATOM	548	ND2	ASN	67	43.947	19.692	39.086	1.00	23.23	AAAA
ATOM	549	C	ASN	67	40.970	23.500	38.250	1.00	15.87	AAAA
ATOM	550	O	ASN	67	41.431	24.347	37.473	1.00	18.64	AAAA
ATOM	551	N	THR	68	39.681	23.180	38.295	1.00	16.55	AAAA
ATOM	552	CA	THR	68	38.729	23.814	37.400	1.00	20.34	AAAA
ATOM	553	CB	THR	68	37.360	23.114	37.441	1.00	22.99	AAAA
ATOM	554	OG1	THR	68	37.511	21.760	36.978	1.00	21.75	AAAA
ATOM	555	CG2	THR	68	36.378	23.827	36.536	1.00	17.37	AAAA
ATOM	556	C	THR	68	38.561	25.291	37.755	1.00	16.66	AAAA
ATOM	557	O	THR	68	38.472	26.139	36.871	1.00	18.79	AAAA
ATOM	558	N	LEU	69	38.534	25.604	39.045	1.00	14.82	AAAA
ATOM	559	CA	LEU	69	38.405	27.000	39.447	1.00	15.20	AAAA
ATOM	560	CB	LEU	69	38.295	27.126	40.973	1.00	16.87	AAAA
ATOM	561	CG	LEU	69	37.057	26.551	41.666	1.00	14.76	AAAA
ATOM	562	CD1	LEU	69	37.212	26.643	43.179	1.00	16.81	AAAA
ATOM	563	CD2	LEU	69	35.832	27.312	41.217	1.00	17.26	AAAA
ATOM	564	C	LEU	69	39.623	27.796	38.969	1.00	15.11	AAAA
ATOM	565	O	LEU	69	39.500	28.934	38.504	1.00	13.30	AAAA
ATOM	566	N	MET	70	40.803	27.204	39.090	1.00	13.40	AAAA
ATOM	567	CA	MET	70	42.019	27.894	38.659	1.00	16.97	AAAA
ATOM	568	CB	MET	70	43.254	27.114	39.075	1.00	14.87	AAAA
ATOM	569	CG	MET	70	43.335	26.886	40.582	1.00	15.18	AAAA
ATOM	570	SD	MET	70	44.828	25.954	41.060	1.00	28.71	AAAA
ATOM	571	CE	MET	70	46.051	27.228	40.893	1.00	21.19	AAAA
ATOM	572	C	MET	70	42.064	28.119	37.155	1.00	19.11	AAAA
ATOM	573	O	MET	70	42.498	29.170	36.700	1.00	17.10	AAAA
ATOM	574	N	GLU	71	41.648	27.118	36.389	1.00	15.06	AAAA
ATOM	575	CA	GLU	71	41.651	27.226	34.934	1.00	16.12	AAAA
ATOM	576	CB	GLU	71	41.397	25.856	34.305	1.00	16.12	AAAA
ATOM	577	CG	GLU	71	41.387	25.882	32.800	1.00	20.26	AAAA
ATOM	578	CD	GLU	71	42.782	25.920	32.193	1.00	32.31	AAAA
ATOM	579	OE1	GLU	71	42.893	25.741	30.958	1.00	27.07	AAAA
ATOM	580	OE2	GLU	71	43.762	26.117	32.941	1.00	24.85	AAAA
ATOM	581	C	GLU	71	40.580	28.208	34.466	1.00	16.48	AAAA
ATOM	582	O	GLU	71	40.831	29.066	33.611	1.00	17.20	AAAA
ATOM	583	N	ALA	72	39.380	28.097	35.027	1.00	15.68	AAAA
ATOM	584	CA	ALA	72	38.300	28.998	34.644	1.00	16.07	AAAA
ATOM	585	CB	ALA	72	37.035	28.669	35.425	1.00	17.21	AAAA
ATOM	586	C	ALA	72	38.678	30.453	34.897	1.00	19.07	AAAA
ATOM	587	O	ALA	72	38.448	31.326	34.054	1.00	15.92	AAAA
ATOM	588	N	GLU	73	39.260	30.726	36.062	1.00	15.86	AAAA
ATOM	589	CA	GLU	73	39.616	32.097	36.372	1.00	15.50	AAAA
ATOM	590	CB	GLU	73	40.046	32.210	37.828	1.00	14.12	AAAA
ATOM	591	CG	GLU	73	40.430	33.615	38.214	1.00	14.24	AAAA
ATOM	592	CD	GLU	73	40.961	33.699	39.629	1.00	17.23	AAAA
ATOM	593	OE1	GLU	73	40.147	33.696	40.573	1.00	18.51	AAAA
ATOM	594	OE2	GLU	73	42.201	33.753	39.793	1.00	20.88	AAAA

Figure 16-10

ATOM	595	C	GLU	73	40.706	32.709	35.495	1.00	20.36	AAAA
ATOM	596	O	GLU	73	40.527	33.806	34.948	1.00	17.74	AAAA
ATOM	597	N	ARG	74	41.832	32.020	35.344	1.00	21.57	AAAA
ATOM	598	CA	ARG	74	42.911	32.623	34.574	1.00	19.48	AAAA
ATOM	599	CB	ARG	74	44.256	31.912	34.834	1.00	18.48	AAAA
ATOM	600	CG	ARG	74	44.365	30.489	34.351	1.00	14.96	AAAA
ATOM	601	CD	ARG	74	45.723	29.892	34.745	1.00	15.05	AAAA
ATOM	602	NE	ARG	74	45.918	28.696	33.950	1.00	18.16	AAAA
ATOM	603	CZ	ARG	74	46.439	28.682	32.727	1.00	16.31	AAAA
ATOM	604	NH1	ARG	74	46.843	29.811	32.145	1.00	19.74	AAAA
ATOM	605	NH2	ARG	74	46.466	27.536	32.047	1.00	14.73	AAAA
ATOM	606	C	ARG	74	42.643	32.718	33.084	1.00	16.86	AAAA
ATOM	607	O	ARG	74	43.148	33.621	32.426	1.00	15.41	AAAA
ATOM	608	N	CYS	75	41.859	31.794	32.547	1.00	17.56	AAAA
ATOM	609	CA	CYS	75	41.544	31.833	31.115	1.00	18.24	AAAA
ATOM	610	CB	CYS	75	41.474	30.414	30.545	1.00	20.94	AAAA
ATOM	611	SG	CYS	75	43.047	29.514	30.572	1.00	19.30	AAAA
ATOM	612	C	CYS	75	40.216	32.561	30.898	1.00	15.81	AAAA
ATOM	613	O	CYS	75	39.762	32.748	29.762	1.00	17.79	AAAA
ATOM	614	N	GLN	76	39.601	32.959	32.007	1.00	15.63	AAAA
ATOM	615	CA	GLN	76	38.339	33.686	32.010	1.00	23.22	AAAA
ATOM	616	CB	GLN	76	38.595	35.122	31.530	1.00	22.99	AAAA
ATOM	617	CG	GLN	76	37.564	36.107	32.027	1.00	44.69	AAAA
ATOM	618	CD	GLN	76	37.588	36.229	33.535	1.00	47.78	AAAA
ATOM	619	OE1	GLN	76	37.563	35.228	34.243	1.00	62.95	AAAA
ATOM	620	NE2	GLN	76	37.619	37.452	34.033	1.00	45.96	AAAA
ATOM	621	C	GLN	76	37.304	32.975	31.135	1.00	23.43	AAAA
ATOM	622	O	GLN	76	36.826	33.512	30.135	1.00	19.93	AAAA
ATOM	623	N	CYS	77	36.951	31.754	31.521	1.00	15.97	AAAA
ATOM	624	CA	CYS	77	36.004	30.979	30.741	1.00	18.91	AAAA
ATOM	625	CB	CYS	77	36.738	30.225	29.623	1.00	24.64	AAAA
ATOM	626	SG	CYS	77	37.848	28.887	30.269	1.00	25.26	AAAA
ATOM	627	C	CYS	77	35.302	29.951	31.594	1.00	19.68	AAAA
ATOM	628	O	CYS	77	35.685	29.702	32.732	1.00	20.02	AAAA
ATOM	629	N	VAL	78	34.254	29.366	31.022	1.00	16.00	AAAA
ATOM	630	CA	VAL	78	33.531	28.288	31.671	1.00	18.73	AAAA
ATOM	631	CB	VAL	78	32.016	28.455	31.557	1.00	15.57	AAAA
ATOM	632	CG1	VAL	78	31.312	27.304	32.262	1.00	21.27	AAAA
ATOM	633	CG2	VAL	78	31.603	29.792	32.151	1.00	19.47	AAAA
ATOM	634	C	VAL	78	33.950	27.077	30.859	1.00	24.02	AAAA
ATOM	635	O	VAL	78	33.499	26.894	29.718	1.00	24.08	AAAA
ATOM	636	N	PRO	79	34.848	26.249	31.420	1.00	18.91	AAAA
ATOM	637	CD	PRO	79	35.470	26.341	32.756	1.00	17.70	AAAA
ATOM	638	CA	PRO	79	35.320	25.056	30.720	1.00	23.37	AAAA
ATOM	639	CB	PRO	79	36.295	24.432	31.732	1.00	21.92	AAAA
ATOM	640	CG	PRO	79	36.802	25.677	32.498	1.00	20.90	AAA
ATOM	641	C	PRO	79	34.152	24.144	30.376	1.00	27.44	AAA
ATOM	642	O	PRO	79	33.177	24.064	31.119	1.00	22.20	AAA
ATOM	643	N	LYS	80	34.245	23.488	29.224	1.00	23.35	AAAA
ATOM	644	CA	LYS	80	33.212	22.570	28.775	1.00	26.78	AAAA
ATOM	645	CB	LYS	80	33.708	21.853	27.518	1.00	32.33	AAAA
ATOM	646	CG	LYS	80	35.098	21.256	27.680	1.00	51.34	AAAA
ATOM	647	CD	LYS	80	35.669	20.817	26.336	1.00	68.70	AAAA
ATOM	648	CE	LYS	80	37.131	20.401	26.451	1.00	70.04	AAAA
ATOM	649	NZ	LYS	80	37.688	19.949	25.141	1.00	73.72	AAAA
ATOM	650	C	LYS	80	32.875	21.571	29.875	1.00	24.71	AAAA
ATOM	651	O	LYS	80	33.770	20.957	30.458	1.00	24.23	AAAA
ATOM	652	N	GLY	81	31.582	21.431	30.161	1.00	16.74	AAAA
ATOM	653	CA	GLY	81	31.126	20.509	31.194	1.00	18.96	AAAA
ATOM	654	C	GLY	81	31.151	21.039	32.630	1.00	22.38	AAAA
ATOM	655	O	GLY	81	30.604	20.396	33.527	1.00	19.29	AAAA
ATOM	656	N	ALA	82	31.754	22.202	32.863	1.00	22.57	AAAA
ATOM	657	CA	ALA	82	31.858	22.738	34.235	1.00	20.65	AAAA
ATOM	658	CB	ALA	82	33.065	23.704	34.333	1.00	20.41	AAAA
ATOM	659	C	ALA	82	30.610	23.425	34.781	1.00	21.81	AAAA
ATOM	660	O	ALA	82	30.425	23.529	35.994	1.00	16.95	AAAA

29/263

Figure 16-11

ATCM	661	N	ARG	83	29.758	23.926	33.897	1.00	17.68	AAAA
ATCM	662	CA	ABG	83	28.549	24.596	34.360	1.00	15.04	AAAA
ATCM	663	CB	ARG	83	27.777	25.188	33.176	1.00	21.02	AAAA
ATCM	664	CG	ARG	83	26.938	26.395	33.528	1.00	36.77	AAAA
ATCM	665	CD	ARG	83	26.061	26.167	34.729	1.00	41.28	AAAA
ATCM	666	NE	ARG	83	25.366	27.393	35.105	1.00	40.05	AAAA
ATCM	667	CZ	ARG	83	24.530	27.492	36.134	1.00	51.15	AAAA
ATCM	668	NH1	ARG	83	24.286	26.432	36.893	1.00	55.10	AAAA
ATCM	669	NH2	ARG	83	23.931	28.646	36.399	1.00	54.26	AAAA
ATCM	670	C	ARG	83	27.701	23.530	35.030	1.00	21.33	AAAA
ATCM	671	O	ARG	83	27.193	23.708	36.130	1.00	24.88	AAAA
ATCM	672	N	GLU	84	27.565	22.406	34.352	1.00	18.76	AAAA
ATCM	673	CA	GLU	84	26.768	21.299	34.859	1.00	24.12	AAAA
ATCM	674	CB	GLU	84	26.527	20.290	33.744	1.00	32.64	AAAA
ATCM	675	CG	GLU	84	27.769	19.994	32.925	1.00	37.91	AAAA
ATCM	676	CD	GLU	84	27.832	20.784	31.612	1.00	51.24	AAAA
ATCM	677	OE1	GLU	84	27.585	20.152	30.545	1.00	24.82	AAAA
ATCM	678	OE2	GLU	84	28.114	22.018	31.650	1.00	22.57	AAAA
ATCM	679	C	GLU	84	27.394	20.570	36.043	1.00	25.36	AAAA
ATCM	680	O	GLU	84	26.739	20.321	37.057	1.00	26.17	AAAA
ATCM	681	N	LYS	85	28.665	20.232	35.897	1.00	18.78	AAAA
ATCM	682	CA	LYS	85	29.399	19.497	36.915	1.00	20.03	AAAA
ATCM	683	CB	LYS	85	30.658	18.900	36.280	1.00	18.59	AAAA
ATCM	684	CG	LYS	85	31.603	18.223	37.268	1.00	35.69	AAAA
ATCM	685	CD	LYS	85	31.151	16.832	37.644	1.00	51.51	AAAA
ATCM	686	CE	LYS	85	31.451	15.864	36.520	1.00	59.18	AAAA
ATCM	687	NZ	LYS	85	32.914	15.858	36.240	1.00	56.63	AAAA
ATCM	688	C	LYS	85	29.811	20.263	38.181	1.00	18.31	AAAA
ATCM	689	O	LYS	85	29.696	19.738	39.290	1.00	21.65	AAAA
ATCM	690	N	TYR	86	30.274	21.495	38.012	1.00	19.45	AAAA
ATCM	691	CA	TYR	86	30.776	22.272	39.145	1.00	14.26	AAAA
ATCM	692	CB	TYR	86	32.207	22.692	38.840	1.00	14.95	AAAA
ATCM	693	CG	TYR	86	33.107	21.508	38.585	1.00	19.76	AAAA
ATCM	694	CD1	TYR	86	33.384	20.591	39.601	1.00	18.83	AAAA
ATCM	695	CE1	TYR	86	34.247	19.519	39.388	1.00	20.29	AAAA
ATCM	696	CD2	TYR	86	33.711	21.322	37.337	1.00	18.14	AAAA
ATCM	697	CE2	TYR	86	34.567	20.261	37.112	1.00	22.66	AAAA
ATCM	698	CZ	TYR	86	34.832	19.364	38.145	1.00	22.61	AAAA
ATCM	699	OH	TYR	86	35.680	18.317	37.921	1.00	23.68	AAAA
ATCM	700	C	TYR	86	29.967	23.493	39.526	1.00	19.03	AAAA
ATCM	701	O	TYR	86	30.353	24.226	40.450	1.00	19.18	AAAA
ATCM	702	N	ASN	87	28.873	23.721	38.803	1.00	17.59	AAAA
ATCM	703	CA	ASN	87	27.953	24.843	39.071	1.00	18.07	AAAA
ATCM	704	CB	ASN	87	27.413	24.730	40.514	1.00	23.87	AAAA
ATCM	705	CG	ASN	87	26.020	25.349	40.688	1.00	30.67	AAAA
ATCM	706	OD1	ASN	87	25.531	25.520	41.819	1.00	31.55	AAAA
ATCM	707	ND2	ASN	87	25.370	25.661	39.580	1.00	20.18	AAAA
ATCM	708	C	ASN	87	28.641	26.197	38.875	1.00	24.24	AAAA
ATCM	709	O	ASN	87	28.283	27.190	39.519	1.00	18.57	AAAA
ATCM	710	N	ILE	88	29.617	26.237	37.970	1.00	18.80	AAAA
ATCM	711	CA	ILE	88	30.353	27.471	37.680	1.00	18.55	AAAA
ATCM	712	CB	ILE	88	31.865	27.166	37.508	1.00	26.44	AAAA
ATCM	713	CG2	ILE	88	32.613	28.406	37.044	1.00	43.71	AAAA
ATCM	714	CG1	ILE	88	32.439	26.703	38.835	1.00	36.30	AAAA
ATCM	715	CD1	ILE	88	32.295	27.735	39.888	1.00	24.08	AAAA
ATCM	716	C	ILE	88	29.887	28.142	36.392	1.00	14.36	AAAA
ATCM	717	O	ILE	88	29.584	27.459	35.426	1.00	21.93	AAAA
ATCM	718	N	GLY	89	29.843	29.473	36.380	1.00	18.71	AAAA
ATCM	719	CA	GLY	89	29.479	30.162	35.154	1.00	20.23	AAAA
ATCM	720	C	GLY	89	28.147	30.873	35.106	1.00	20.85	AAAA
ATCM	721	O	GLY	89	28.006	31.817	34.330	1.00	25.47	AAAA
ATCM	722	N	GLY	90	27.172	30.414	35.889	1.00	21.17	AAAA
ATCM	723	CA	GLY	90	25.863	31.060	35.898	1.00	24.44	AAAA
ATCM	724	C	GLY	90	25.862	32.371	36.668	1.00	30.60	AAAA
ATCM	725	O	GLY	90	26.900	32.788	37.168	1.00	28.13	AAAA
ATCM	726	N	TYR	91	24.708	33.036	36.755	1.00	23.38	AAAA

30/263 Figure 16-12

ATOM	727	CA	TYR	91	24.598	34.299	37.490	1.00	28.48	AAAA
ATOM	728	CB	TYR	91	23.144	34.753	37.545	1.00	29.88	AAAA
ATOM	729	CG	TYR	91	22.923	35.899	38.518	1.00	33.88	AAAA
ATOM	730	CD1	TYR	91	23.329	37.197	38.207	1.00	39.69	AAAA
ATOM	731	CE1	TYR	91	23.130	38.250	39.104	1.00	31.76	AAAA
ATOM	732	CD2	TYR	91	22.317	35.678	39.759	1.00	40.63	AAAA
ATOM	733	CE2	TYR	91	22.115	36.720	40.664	1.00	37.07	AAAA
ATOM	734	CZ	TYR	91	22.521	38.002	40.327	1.00	36.22	AAAA
ATOM	735	OH	TYR	91	22.306	39.035	41.210	1.00	44.71	AAAA
ATOM	736	C	TYR	91	25.075	34.157	38.937	1.00	23.59	AAAA
ATOM	737	O	TYR	91	25.713	35.041	39.502	1.00	22.64	AAAA
ATOM	738	N	GLU	92	24.724	33.032	39.531	1.00	23.09	AAAA
ATOM	739	CA	GLU	92	25.048	32.747	40.917	1.00	26.61	AAAA
ATOM	740	CB	GLU	92	24.289	31.476	41.306	1.00	32.57	AAAA
ATOM	741	CG	GLU	92	24.595	30.892	42.657	1.00	41.38	AAAA
ATOM	742	CD	GLU	92	23.604	29.800	43.023	1.00	49.02	AAAA
ATOM	743	OE1	GLU	92	24.008	28.829	43.715	1.00	45.51	AAAA
ATOM	744	OE2	GLU	92	22.418	29.931	42.628	1.00	38.16	AAAA
ATOM	745	C	GLU	92	26.541	32.636	41.251	1.00	25.78	AAAA
ATOM	746	O	GLU	92	27.045	33.358	42.125	1.00	24.95	AAAA
ATOM	747	N	ASN	93	27.243	31.742	40.556	1.00	21.41	AAAA
ATOM	748	CA	ASN	93	28.674	31.519	40.777	1.00	21.14	AAAA
ATOM	749	CB	ASN	93	28.876	30.075	41.226	1.00	17.27	AAAA
ATOM	750	CG	ASN	93	27.905	29.682	42.320	1.00	15.34	AAAA
ATOM	751	OD1	ASN	93	27.882	30.290	43.399	1.00	20.33	AAAA
ATOM	752	ND2	ASN	93	27.078	28.674	42.047	1.00	20.49	AAAA
ATOM	753	C	ASN	93	29.378	31.778	39.445	1.00	22.25	AAAA
ATOM	754	O	ASN	93	29.901	30.865	38.806	1.00	20.29	AAAA
ATOM	755	N	PRO	94	29.451	33.057	39.045	1.00	25.45	AAAA
ATOM	756	CD	PRO	94	29.027	34.221	39.839	1.00	23.03	AAAA
ATOM	757	CA	PRO	94	30.055	33.523	37.794	1.00	23.05	AAAA
ATOM	758	CB	PRO	94	29.669	35.004	37.759	1.00	28.71	AAAA
ATOM	759	CG	PRO	94	28.528	35.112	38.755	1.00	40.02	AAAA
ATOM	760	C	PRO	94	31.554	33.384	37.697	1.00	26.51	AAAA
ATOM	761	O	PRO	94	32.232	33.185	38.688	1.00	17.36	AAAA
ATOM	762	N	VAL	95	32.068	33.498	36.478	1.00	21.12	AAAA
ATOM	763	CA	VAL	95	33.506	33.493	36.281	1.00	17.00	AAAA
ATOM	764	CB	VAL	95	33.851	33.242	34.796	1.00	25.15	AAAA
ATOM	765	CG1	VAL	95	35.326	33.537	34.533	1.00	27.19	AAAA
ATOM	766	CG2	VAL	95	33.551	31.791	34.443	1.00	17.37	AAAA
ATOM	767	C	VAL	95	33.989	34.899	36.686	1.00	17.42	AAAA
ATOM	768	O	VAL	95	33.426	35.894	36.237	1.00	23.43	AAAA
ATOM	769	N	SER	96	34.986	34.982	37.563	1.00	18.84	AAAA
ATOM	770	CA	SER	96	35.564	36.270	37.982	1.00	21.77	AAAA
ATOM	771	CB	SER	96	34.608	37.070	38.867	1.00	23.11	AAAA
ATOM	772	OG	SER	96	34.723	36.679	40.223	1.00	24.43	AAAA
ATOM	773	C	SER	96	36.835	35.987	38.789	1.00	29.09	AAAA
ATOM	774	O	SER	96	37.117	34.828	39.115	1.00	27.12	AAAA
ATOM	775	N	TYR	97	37.610	37.020	39.124	1.00	17.51	AAAA
ATOM	776	CA	TYR	97	38.803	36.751	39.911	1.00	20.69	AAAA
ATOM	777	CB	TYR	97	39.865	37.835	39.712	1.00	21.82	AAAA
ATOM	778	CG	TYR	97	40.492	37.748	38.332	1.00	22.72	AAAA
ATOM	779	CD1	TYR	97	39.936	38.414	37.235	1.00	28.47	AAAA
ATOM	780	CE1	TYR	97	40.473	38.265	35.949	1.00	24.45	AAAA
ATOM	781	CD2	TYR	97	41.599	36.929	38.112	1.00	19.74	AAAA
ATOM	782	CE2	TYR	97	42.144	36.771	36.832	1.00	21.63	AAAA
ATOM	783	CZ	TYR	97	41.578	37.439	35.759	1.00	23.13	AAAA
ATOM	784	OH	TYR	97	42.122	37.273	34.501	1.00	28.54	AAAA
ATOM	785	C	TYR	97	38.510	36.515	41.393	1.00	20.12	AAAA
ATOM	786	O	TYR	97	39.413	36.285	42.194	1.00	19.76	AAAA
ATOM	787	N	ALA	98	37.243	36.558	41.764	1.00	18.56	AAAA
ATOM	788	CA	ALA	98	36.899	36.259	43.139	1.00	22.23	AAAA
ATOM	789	CB	ALA	98	35.561	36.888	43.515	1.00	27.92	AAAA
ATOM	790	C	ALA	98	36.776	34.743	43.224	1.00	23.56	AAAA
ATOM	791	O	ALA	98	36.931	34.166	44.289	1.00	20.14	AAAA
ATOM	792	N	MET	99	36.538	34.094	42.087	1.00	16.84	AAAA

31/263 Figure 16-13

ATOM	793	CA	MET	99	36.295	32.643	42.117	1.00	17.60	AAAA
ATOM	794	CB	MET	99	35.864	32.137	40.736	1.00	17.05	AAAA
ATOM	795	CG	MET	99	36.999	31.824	39.793	1.00	11.16	AAAA
ATOM	796	SD	MET	99	36.314	31.698	38.113	1.00	16.54	AAAA
ATOM	797	CE	MET	99	35.165	30.295	38.312	1.00	17.83	AAAA
ATOM	798	C	MET	99	37.432	31.800	42.650	1.00	18.98	AAAA
ATOM	799	O	MET	99	37.197	30.753	43.251	1.00	18.21	AAAA
ATOM	800	N	PHE	100	38.670	32.216	42.420	1.00	12.87	AAAA
ATOM	801	CA	PHE	100	39.774	31.439	42.987	1.00	17.13	AAAA
ATOM	802	CB	PHE	100	40.559	30.681	41.917	1.00	15.23	AAAA
ATOM	803	CG	PHE	100	41.647	29.834	42.492	1.00	15.20	AAAA
ATOM	804	CD1	PHE	100	41.342	28.638	43.140	1.00	22.96	AAAA
ATOM	805	CD2	PHE	100	42.972	30.282	42.488	1.00	17.12	AAAA
ATOM	806	CE1	PHE	100	42.341	27.901	43.782	1.00	19.23	AAAA
ATOM	807	CE2	PHE	100	43.974	29.552	43.129	1.00	16.99	AAAA
ATOM	808	CZ	PHE	100	43.658	28.360	43.779	1.00	17.78	AAAA
ATOM	809	C	PHE	100	40.755	32.305	43.774	1.00	20.54	AAAA
ATOM	810	O	PHE	100	41.088	31.990	44.912	1.00	21.45	AAAA
ATOM	811	N	THR	101	41.219	33.401	43.187	1.00	18.02	AAAA
ATOM	812	CA	THR	101	42.177	34.245	43.902	1.00	15.25	AAAA
ATOM	813	CB	THR	101	42.715	35.341	42.976	1.00	16.33	AAAA
ATOM	814	OG1	THR	101	43.386	34.720	41.870	1.00	16.01	AAAA
ATOM	815	CG2	THR	101	43.706	36.226	43.697	1.00	16.31	AAAA
ATOM	816	C	THR	101	41.567	34.860	45.160	1.00	14.12	AAAA
ATOM	817	O	THR	101	42.110	34.707	46.244	1.00	16.86	AAAA
ATOM	818	N	GLY	102	40.435	35.541	45.008	1.00	13.77	AAAA
ATOM	819	CA	GLY	102	39.770	36.145	46.156	1.00	16.29	AAAA
ATOM	820	C	GLY	102	39.330	35.065	47.133	1.00	16.75	AAAA
ATOM	821	O	GLY	102	39.502	35.202	48.338	1.00	14.48	AAAA
ATOM	822	N	SER	103	38.752	33.986	46.615	1.00	16.24	AAAA
ATOM	823	CA	SER	103	38.315	32.890	47.488	1.00	16.72	AAAA
ATOM	824	CB	SER	103	37.567	31.821	46.684	1.00	15.97	AAAA
ATOM	825	OG	SER	103	36.339	32.349	46.197	1.00	26.86	AAAA
ATOM	826	C	SER	103	39.494	32.264	48.218	1.00	17.88	AAAA
ATOM	827	O	SER	103	39.405	31.974	49.419	1.00	14.17	AAAA
ATOM	828	N	SER	104	40.604	32.057	47.515	1.00	11.40	AAAA
ATOM	829	CA	SER	104	41.780	31.484	48.181	1.00	17.61	AAAA
ATOM	830	CB	SER	104	42.888	31.206	47.160	1.00	15.89	AAAA
ATOM	831	OG	SER	104	42.525	30.102	46.362	1.00	27.82	AAAA
ATOM	832	C	SER	104	42.332	32.404	49.271	1.00	17.02	AAAA
ATOM	833	O	SER	104	42.867	31.958	50.286	1.00	15.37	AAAA
ATOM	834	N	LEU	105	42.206	33.698	49.052	1.00	17.10	AAAA
ATOM	835	CA	LEU	105	42.709	34.652	50.016	1.00	16.95	AAAA
ATOM	836	CB	LEU	105	42.728	36.037	49.365	1.00	18.44	AAAA
ATOM	837	CG	LEU	105	43.613	37.108	49.981	1.00	29.88	AAAA
ATOM	838	CD1	LEU	105	45.086	36.631	49.959	1.00	20.25	AAAA
ATOM	839	CD2	LEU	105	43.438	38.418	49.175	1.00	29.39	AAAA
ATOM	840	C	LEU	105	41.837	34.637	51.282	1.00	14.81	AAAA
ATOM	841	O	LEU	105	42.334	34.703	52.404	1.00	17.74	AAAA
ATOM	842	N	ALA	106	40.532	34.531	51.095	1.00	19.28	AAAA
ATOM	843	CA	ALA	106	39.601	34.493	52.224	1.00	12.39	AAAA
ATOM	844	CB	ALA	106	38.140	34.574	51.704	1.00	11.58	AAAA
ATOM	845	C	ALA	106	39.807	33.210	53.023	1.00	14.79	AAAA
ATOM	846	O	ALA	106	39.704	33.203	54.250	1.00	13.58	AAAA
ATOM	847	N	THR	107	40.114	32.128	52.318	1.00	13.67	AAAA
ATOM	848	CA	THR	107	40.314	30.819	52.956	1.00	13.21	AAAA
ATOM	849	CB	THR	107	40.187	29.708	51.902	1.00	14.95	AAAA
ATOM	850	OG1	THR	107	38.868	29.792	51.334	1.00	15.72	AAAA
ATOM	851	CG2	THR	107	40.422	28.311	52.511	1.00	9.51	AAAA
ATOM	852	C	THR	107	41.649	30.751	53.687	1.00	15.80	AAAA
ATOM	853	O	THR	107	41.734	30.206	54.792	1.00	15.63	AAAA
ATOM	854	N	GLY	108	42.696	31.294	53.082	1.00	14.08	AAAA
ATOM	855	CA	GLY	108	43.968	31.298	53.765	1.00	14.62	AAAA
ATOM	856	C	GLY	108	43.801	32.119	55.041	1.00	20.05	AAAA
ATOM	857	O	GLY	108	44.417	31.813	56.063	1.00	17.53	AAAA
ATOM	858	N	SER	109	42.963	33.158	54.988	1.00	15.26	AAAA

32/263

Figure 16-14

ATOM	859	CA	SER	109	42.727	34.020	56.153	1.00	14.54	AAAA
ATOM	860	CB	SER	109	41.906	35.248	55.737	1.00	15.58	AAAA
ATOM	861	OG	SER	109	42.627	36.045	54.809	1.00	16.97	AAAA
ATOM	862	C	SER	109	42.037	33.264	57.297	1.00	15.56	AAAA
ATOM	863	O	SER	109	42.189	33.600	58.487	1.00	17.00	AAAA
ATOM	864	N	THR	110	41.261	32.247	56.944	1.00	14.37	AAAA
ATOM	865	CA	THR	110	40.608	31.435	57.957	1.00	12.89	AAAA
ATOM	866	CB	THR	110	39.452	30.628	57.360	1.00	14.54	AAAA
ATOM	867	OG1	THR	110	38.346	31.519	57.163	1.00	18.11	AAAA
ATOM	868	CG2	THR	110	39.061	29.452	58.278	1.00	12.91	AAAA
ATOM	869	C	THR	110	41.633	30.524	58.601	1.00	18.44	AAAA
ATOM	870	O	THR	110	41.574	30.302	59.806	1.00	16.30	AAAA
ATOM	871	N	VAL	111	42.584	30.013	57.816	1.00	15.20	AAAA
ATOM	872	CA	VAL	111	43.614	29.180	58.403	1.00	20.45	AAAA
ATOM	873	CB	VAL	111	44.517	28.514	57.323	1.00	20.02	AAAA
ATOM	874	CG1	VAL	111	45.652	27.765	58.005	1.00	21.79	AAAA
ATOM	875	CG2	VAL	111	43.697	27.537	56.482	1.00	19.07	AAAA
ATOM	876	C	VAL	111	44.456	30.075	59.327	1.00	18.21	AAAA
ATOM	877	O	VAL	111	44.838	29.672	60.431	1.00	18.65	AAAA
ATOM	878	N	GLN	112	44.731	31.302	58.890	1.00	16.82	AAAA
ATOM	879	CA	GLN	112	45.493	32.232	59.719	1.00	20.13	AAAA
ATOM	880	CB	GLN	112	45.751	33.540	58.970	1.00	22.39	AAAA
ATOM	881	CG	GLN	112	46.593	33.360	57.723	1.00	21.17	AAAA
ATOM	882	CD	GLN	112	46.797	34.651	56.982	1.00	24.82	AAAA
ATOM	883	OE1	GLN	112	47.772	35.381	57.219	1.00	25.62	AAAA
ATOM	884	NE2	GLN	112	45.866	34.963	56.091	1.00	13.16	AAAA
ATOM	885	C	GLN	112	44.743	32.516	61.012	1.00	23.99	AAAA
ATOM	886	O	GLN	112	45.340	32.593	62.079	1.00	17.94	AAAA
ATOM	887	N	ALA	113	43.431	32.700	60.924	1.00	15.60	AAAA
ATOM	888	CA	ALA	113	42.653	32.941	62.138	1.00	15.04	AAAA
ATOM	889	CB	ALA	113	41.191	33.138	61.802	1.00	18.65	AAAA
ATOM	890	C	ALA	113	42.807	31.751	63.083	1.00	14.84	AAAA
ATOM	891	O	ALA	113	42.941	31.909	64.296	1.00	21.05	AAAA
ATOM	892	N	ILE	114	42.767	30.550	62.534	1.00	16.45	AAAA
ATOM	893	CA	ILE	114	42.919	29.383	63.389	1.00	15.38	AAAA
ATOM	894	CB	ILE	114	42.600	28.100	62.637	1.00	15.22	AAAA
ATOM	895	CG2	ILE	114	42.888	26.893	63.537	1.00	15.72	AAAA
ATOM	896	CG1	ILE	114	41.110	28.112	62.244	1.00	19.28	AAAA
ATOM	897	CD1	ILE	114	40.744	27.038	61.191	1.00	13.43	AAAA
ATOM	898	C	ILE	114	44.329	29.318	63.968	1.00	18.02	AAAA
ATOM	899	O	ILE	114	44.508	28.998	65.156	1.00	20.38	AAAA
ATOM	900	N	GLU	115	45.328	29.629	63.144	1.00	15.27	AAAA
ATOM	901	CA	GLU	115	46.726	29.626	63.614	1.00	21.48	AAAA
ATOM	902	CB	GLU	115	47.690	30.080	62.506	1.00	21.76	AAAA
ATOM	903	CG	GLU	115	47.884	29.080	61.386	1.00	15.78	AAAA
ATOM	904	CD	GLU	115	48.670	29.648	60.211	1.00	20.04	AAAA
ATOM	905	OE1	GLU	115	49.051	30.843	60.239	1.00	21.48	AAAA
ATOM	906	OE2	GLU	115	48.901	28.902	59.241	1.00	26.59	AAAA
ATOM	907	C	GLU	115	46.877	30.559	64.814	1.00	23.55	AAAA
ATOM	908	O	GLU	115	47.509	30.212	65.815	1.00	23.03	AAAA
ATOM	909	N	GLU	116	46.295	31.748	64.703	1.00	22.73	AAAA
ATOM	910	CA	GLU	116	46.367	32.735	65.774	1.00	20.54	AAAA
ATOM	911	CB	GLU	116	45.744	34.044	65.320	1.00	18.40	AAAA
ATOM	912	CG	GLU	116	46.562	34.765	64.279	1.00	19.76	AAAA
ATOM	913	CD	GLU	116	47.985	34.998	64.756	1.00	27.24	AAAA
ATOM	914	OE1	GLU	116	48.164	35.630	65.815	1.00	18.44	AAAA
ATOM	915	OE2	GLU	116	48.919	34.543	64.078	1.00	23.17	AAAA
ATOM	916	C	GLU	116	45.682	32.253	67.034	1.00	25.39	AAAA
ATOM	917	O	GLU	116	46.207	32.427	68.137	1.00	22.87	AAAA
ATOM	918	N	PHE	117	44.510	31.647	66.872	1.00	18.78	AAAA
ATOM	919	CA	PHE	117	43.778	31.139	68.019	1.00	22.11	AAAA
ATOM	920	CB	PHE	117	42.451	30.530	67.581	1.00	23.14	AAAA
ATOM	921	CG	PHE	117	41.603	30.054	68.728	1.00	24.06	AAAA
ATOM	922	CD1	PHE	117	40.880	30.961	69.493	1.00	19.67	AAAA
ATOM	923	CD2	PHE	117	41.559	28.701	69.066	1.00	24.08	AAAA
ATOM	924	CE1	PHE	117	40.115	30.531	70.586	1.00	23.68	AAAA

ATOM	925	CE2	PHE	117	40.799	28.262	70.156	1.00	24.04	AAAA
ATOM	926	CZ	PHE	117	40.078	29.179	70.915	1.00	19.62	AAAA
ATOM	927	C	PHE	117	44.587	30.068	68.747	1.00	23.87	AAAA
ATOM	928	O	PHE	117	44.613	30.031	69.979	1.00	24.40	AAAA
ATOM	929	N	LEU	118	45.238	29.194	67.981	1.00	21.09	AAAA
ATOM	930	CA	LEU	118	46.025	28.113	68.549	1.00	20.73	AAAA
ATOM	931	CB	LEU	118	46.358	27.075	67.480	1.00	17.90	AAAA
ATOM	932	CG	LEU	118	45.148	26.264	66.984	1.00	26.20	AAAA
ATOM	933	CD1	LEU	118	45.591	25.288	65.924	1.00	34.23	AAAA
ATOM	934	CD2	LEU	118	44.520	25.499	68.139	1.00	27.16	AAAA
ATOM	935	C	LEU	118	47.290	28.601	69.238	1.00	26.49	AAAA
ATOM	936	O	LEU	118	47.908	27.856	69.996	1.00	26.34	AAAA
ATOM	937	N	LYS	119	47.672	29.848	68.975	1.00	28.92	AAAA
ATOM	938	CA	LYS	119	48.835	30.459	69.624	1.00	28.53	AAAA
ATOM	939	CB	LYS	119	49.392	31.616	68.805	1.00	30.15	AAAA
ATOM	940	CG	LYS	119	49.915	31.267	67.437	1.00	35.14	AAAA
ATOM	941	CD	LYS	119	50.291	32.549	66.716	1.00	28.98	AAAA
ATOM	942	CE	LYS	119	50.905	32.262	65.380	1.00	31.07	AAAA
ATOM	943	NZ	LYS	119	51.195	33.551	64.745	1.00	22.46	AAAA
ATOM	944	C	LYS	119	48.335	31.053	70.932	1.00	35.74	AAAA
ATOM	945	O	LYS	119	49.117	31.541	71.750	1.00	27.10	AAAA
ATOM	946	N	GLY	120	47.018	31.050	71.103	1.00	25.20	AAAA
ATOM	947	CA	GLY	120	46.445	31.605	72.309	1.00	30.18	AAAA
ATOM	948	C	GLY	120	45.913	33.007	72.122	1.00	31.91	AAAA
ATOM	949	O	GLY	120	45.540	33.665	73.094	1.00	34.76	AAAA
ATOM	950	N	ASN	121	45.889	33.495	70.887	1.00	20.56	AAAA
ATOM	951	CA	ASN	121	45.353	34.825	70.681	1.00	25.58	AAAA
ATOM	952	CB	ASN	121	46.278	35.634	69.785	1.00	29.99	AAAA
ATOM	953	CG	ASN	121	47.641	35.827	70.427	1.00	24.43	AAAA
ATOM	954	OD1	ASN	121	48.396	34.874	70.588	1.00	54.63	AAAA
ATOM	955	ND2	ASN	121	47.944	37.045	70.817	1.00	41.69	AAAA
ATOM	956	C	ASN	121	43.941	34.759	70.135	1.00	18.85	AAAA
ATOM	957	O	ASN	121	43.421	33.675	69.899	1.00	24.77	AAAA
ATOM	958	N	VAL	122	43.310	35.918	69.991	1.00	19.55	AAAA
ATOM	959	CA	VAL	122	41.936	35.994	69.499	1.00	22.90	AAAA
ATOM	960	CB	VAL	122	41.053	36.832	70.449	1.00	31.47	AAAA
ATOM	961	CG1	VAL	122	39.649	37.006	69.851	1.00	31.52	AAAA
ATOM	962	CG2	VAL	122	40.986	36.154	71.810	1.00	32.50	AAAA
ATOM	963	C	VAL	122	41.953	36.632	68.130	1.00	16.87	AAAA
ATOM	964	O	VAL	122	42.518	37.710	67.938	1.00	24.08	AAAA
ATOM	965	N	ALA	123	41.321	35.983	67.159	1.00	18.67	AAAA
ATOM	966	CA	ALA	123	41.360	36.532	65.821	1.00	10.18	AAAA
ATOM	967	CB	ALA	123	42.346	35.743	64.990	1.00	19.04	AAAA
ATOM	968	C	ALA	123	40.000	36.551	65.131	1.00	13.72	AAAA
ATOM	969	O	ALA	123	39.108	35.761	65.439	1.00	20.78	AAAA
ATOM	970	N	PHE	124	39.871	37.457	64.180	1.00	12.92	AAAA
ATOM	971	CA	PHE	124	38.649	37.610	63.401	1.00	14.67	AAAA
ATOM	972	CB	PHE	124	37.904	38.878	63.856	1.00	14.67	AAAA
ATOM	973	CG	PHE	124	36.660	39.209	63.049	1.00	20.28	AAAA
ATOM	974	CD1	PHE	124	35.811	38.209	62.587	1.00	18.56	AAAA
ATOM	975	CD2	PHE	124	36.286	40.545	62.843	1.00	19.53	AAAA
ATOM	976	CE1	PHE	124	34.609	38.532	61.937	1.00	18.75	AAAA
ATOM	977	CE2	PHE	124	35.072	40.875	62.193	1.00	20.18	AAAA
ATOM	978	CZ	PHE	124	34.242	39.867	61.744	1.00	21.57	AAAA
ATOM	979	C	PHE	124	39.016	37.712	61.930	1.00	22.60	AAAA
ATOM	980	O	PHE	124	39.823	38.558	61.535	1.00	19.22	AAAA
ATOM	981	N	ASN	125	38.449	36.820	61.126	1.00	19.39	AAAA
ATOM	982	CA	ASN	125	38.651	36.858	59.691	1.00	16.80	AAAA
ATOM	983	CB	ASN	125	39.122	35.507	59.150	1.00	15.71	AAAA
ATOM	984	CG	ASN	125	39.063	35.469	57.649	1.00	12.84	AAAA
ATOM	985	OD1	ASN	125	39.216	36.508	57.006	1.00	14.91	AAAA
ATOM	986	ND2	ASN	125	38.853	34.272	57.065	1.00	16.21	AAAA
ATOM	987	C	ASN	125	37.315	37.210	59.038	1.00	16.22	AAAA
ATOM	988	O	ASN	125	36.502	36.330	58.755	1.00	15.28	AAAA
ATOM	989	N	PRO	126	37.071	38.502	58.775	1.00	14.84	AAAA
ATOM	990	CD	PRO	126	37.908	39.684	59.052	1.00	18.10	AAAA

Figure 16-16

ATOM	991	CA	PRO	126	35.811	38.910	58.156	1.00	17.33	AAAA
ATOM	992	CB	PRO	126	35.912	40.434	58.177	1.00	16.32	AAAA
ATOM	993	CG	PRO	126	37.416	40.655	58.008	1.00	20.95	AAAA
ATOM	994	C	PRO	126	35.549	38.359	56.752	1.00	13.78	AAAA
ATOM	995	O	PRO	126	34.404	38.291	56.322	1.00	17.03	AAAA
ATOM	996	N	ALA	127	36.607	37.972	56.042	1.00	14.57	AAAA
ATOM	997	CA	ALA	127	36.463	37.443	54.691	1.00	17.37	AAAA
ATOM	998	CB	ALA	127	37.816	37.540	53.930	1.00	14.48	AAAA
ATOM	999	C	ALA	127	35.982	35.998	54.702	1.00	19.77	AAAA
ATOM	1000	O	ALA	127	35.490	35.500	53.688	1.00	15.62	AAAA
ATOM	1001	N	GLY	128	36.111	35.339	55.849	1.00	13.54	AAAA
ATOM	1002	CA	GLY	128	35.725	33.939	55.971	1.00	13.53	AAAA
ATOM	1003	C	GLY	128	34.234	33.679	56.101	1.00	14.49	AAAA
ATOM	1004	O	GLY	128	33.414	34.585	56.017	1.00	15.65	AAAA
ATOM	1005	N	GLY	129	33.883	32.420	56.314	1.00	13.35	AAAA
ATOM	1006	CA	GLY	129	32.487	32.058	56.446	1.00	16.28	AAAA
ATOM	1007	C	GLY	129	31.754	31.831	55.130	1.00	15.69	AAAA
ATOM	1008	O	GLY	129	30.543	32.021	55.072	1.00	16.10	AAAA
ATOM	1009	N	MET	130	32.479	31.448	54.079	1.00	15.00	AAAA
ATOM	1010	CA	MET	130	31.879	31.163	52.757	1.00	13.35	AAAA
ATOM	1011	CB	MET	130	32.969	31.215	51.689	1.00	12.20	AAAA
ATOM	1012	CG	MET	130	33.680	32.573	51.731	1.00	17.03	AAAA
ATOM	1013	SD	MET	130	34.863	32.877	50.425	1.00	15.41	AAAA
ATOM	1014	CE	MET	130	33.752	32.973	49.073	1.00	46.82	AAAA
ATOM	1015	C	MET	130	31.296	29.756	52.885	1.00	12.49	AAAA
ATOM	1016	O	MET	130	31.785	28.789	52.297	1.00	19.54	AAAA
ATOM	1017	N	HIS	131	30.188	29.695	53.617	1.00	16.24	AAAA
ATOM	1018	CA	HIS	131	29.556	28.448	54.014	1.00	13.80	AAAA
ATOM	1019	CB	HIS	131	28.772	28.694	55.316	1.00	15.91	AAAA
ATOM	1020	CG	HIS	131	27.606	29.625	55.175	1.00	13.08	AAAA
ATOM	1021	CD2	HIS	131	26.712	30.063	56.096	1.00	12.46	AAAA
ATOM	1022	ND1	HIS	131	27.225	30.190	53.976	1.00	22.48	AAAA
ATOM	1023	CE1	HIS	131	26.148	30.936	54.166	1.00	16.56	AAAA
ATOM	1024	NE2	HIS	131	25.817	30.875	55.442	1.00	23.56	AAAA
ATOM	1025	C	HIS	131	28.673	27.663	53.066	1.00	13.69	AAAA
ATOM	1026	O	HIS	131	28.125	26.658	53.470	1.00	17.21	AAAA
ATOM	1027	N	HIS	132	28.523	28.115	51.830	1.00	14.51	AAAA
ATOM	1028	CA	HIS	132	27.669	27.400	50.887	1.00	20.19	AAAA
ATOM	1029	CB	HIS	132	26.863	28.416	50.054	1.00	17.26	AAAA
ATOM	1030	CG	HIS	132	25.748	29.070	50.810	1.00	16.85	AAAA
ATOM	1031	CD2	HIS	132	24.787	28.542	51.604	1.00	13.74	AAAA
ATOM	1032	ND1	HIS	132	25.497	30.424	50.756	1.00	24.80	AAAA
ATOM	1033	CE1	HIS	132	24.429	30.700	51.486	1.00	12.68	AAAA
ATOM	1034	NE2	HIS	132	23.980	29.576	52.010	1.00	28.65	AAAA
ATOM	1035	C	HIS	132	28.372	26.412	49.946	1.00	16.89	AAAA
ATOM	1036	O	HIS	132	27.731	25.487	49.460	1.00	14.58	AAAA
ATOM	1037	N	ALA	133	29.669	26.580	49.689	1.00	16.79	AAAA
ATOM	1038	CA	ALA	133	30.338	25.680	48.740	1.00	13.76	AAAA
ATOM	1039	CB	ALA	133	31.738	26.194	48.412	1.00	14.95	AAAA
ATOM	1040	C	ALA	133	30.418	24.219	49.179	1.00	18.80	AAAA
ATOM	1041	O	ALA	133	30.557	23.939	50.355	1.00	16.86	AAAA
ATOM	1042	N	PHE	134	30.306	23.306	48.209	1.00	13.76	AAAA
ATOM	1043	CA	PHE	134	30.378	21.868	48.451	1.00	19.77	AAAA
ATOM	1044	CB	PHE	134	29.311	21.132	47.620	1.00	15.59	AAAA
ATOM	1045	CG	PHE	134	27.917	21.525	47.975	1.00	17.22	AAAA
ATOM	1046	CD1	PHE	134	27.135	22.259	47.091	1.00	17.88	AAAA
ATOM	1047	CD2	PHE	134	27.392	21.187	49.222	1.00	21.68	AAAA
ATOM	1048	CE1	PHE	134	25.836	22.653	47.445	1.00	23.07	AAAA
ATOM	1049	CE2	PHE	134	26.099	21.578	49.585	1.00	17.64	AAAA
ATOM	1050	CZ	PHE	134	25.323	22.308	48.696	1.00	19.71	AAAA
ATOM	1051	C	PHE	134	31.763	21.354	48.098	1.00	14.76	AAAA
ATOM	1052	O	PHE	134	32.547	22.049	47.442	1.00	18.05	AAAA
ATOM	1053	N	LYS	135	32.060	20.124	48.515	1.00	16.37	AAAA
ATOM	1054	CA	LYS	135	33.369	19.551	48.269	1.00	16.24	AAAA
ATOM	1055	CB	LYS	135	33.360	18.070	48.699	1.00	21.29	AAAA
ATOM	1056	CG	LYS	135	34.640	17.300	48.400	1.00	30.43	AAAA

Figure 16-17

ATOM	1057	CD	LYS	135	34.597	15.867	48.977	1.00	30.26	AAAA
ATOM	1058	CE	LYS	135	34.862	15.805	50.486	1.00	35.01	AAAA
ATOM	1059	NZ	LYS	135	36.304	16.023	50.895	1.00	20.61	AAAA
ATOM	1060	C	LYS	135	33.854	19.687	46.836	1.00	16.60	AAAA
ATOM	1061	O	LYS	135	35.020	20.020	46.584	1.00	17.24	AAAA
ATOM	1062	N	SER	136	32.944	19.483	45.893	1.00	18.01	AAAA
ATOM	1063	CA	SER	136	33.301	19.528	44.490	1.00	15.26	AAAA
ATOM	1064	CB	SER	136	33.339	18.094	43.940	1.00	18.07	AAAA
ATOM	1065	OG	SER	136	34.135	17.261	44.762	1.00	22.22	AAAA
ATOM	1066	C	SER	136	32.345	20.355	43.658	1.00	15.40	AAAA
ATOM	1067	O	SER	136	32.162	20.071	42.475	1.00	18.77	AAAA
ATOM	1068	N	ARG	137	31.754	21.401	44.237	1.00	19.71	AAAA
ATOM	1069	CA	ARG	137	30.805	22.216	43.482	1.00	17.29	AAAA
ATOM	1070	CB	ARG	137	29.481	21.448	43.366	1.00	24.19	AAAA
ATOM	1071	CG	ARG	137	28.290	22.273	42.937	1.00	32.56	AAAA
ATOM	1072	CD	ARG	137	27.026	21.424	42.980	1.00	47.98	AAAA
ATOM	1073	NE	ARG	137	26.951	20.493	41.862	1.00	50.95	AAAA
ATOM	1074	CZ	ARG	137	26.392	20.781	40.691	1.00	50.38	AAAA
ATOM	1075	NH1	ARG	137	25.854	21.976	40.485	1.00	45.26	AAAA
ATOM	1076	NH2	ARG	137	26.375	19.876	39.722	1.00	55.31	AAAA
ATOM	1077	C	ARG	137	30.537	23.595	44.095	1.00	16.14	AAAA
ATOM	1078	O	ARG	137	30.439	23.711	45.308	1.00	16.88	AAAA
ATOM	1079	N	ALA	138	30.395	24.621	43.252	1.00	18.07	AAAA
ATOM	1080	CA	ALA	138	30.117	25.976	43.735	1.00	21.48	AAAA
ATOM	1081	CB	ALA	138	30.460	27.024	42.631	1.00	16.55	AAAA
ATOM	1082	C	ALA	138	28.642	26.090	44.135	1.00	21.04	AAAA
ATOM	1083	O	ALA	138	27.798	25.339	43.641	1.00	18.97	AAAA
ATOM	1084	N	ASN	139	28.321	27.019	45.029	1.00	13.83	AAAA
ATOM	1085	CA	ASN	139	26.952	27.158	45.468	1.00	12.92	AAAA
ATOM	1086	CB	ASN	139	26.566	25.899	46.274	1.00	13.14	AAAA
ATOM	1087	CG	ASN	139	25.162	25.961	46.832	1.00	20.34	AAAA
ATOM	1088	OD1	ASN	139	24.186	26.068	46.086	1.00	19.76	AAAA
ATOM	1089	ND2	ASN	139	25.048	25.881	48.157	1.00	16.36	AAAA
ATOM	1090	C	ASN	139	26.756	28.409	46.315	1.00	20.92	AAAA
ATOM	1091	O	ASN	139	27.603	28.738	47.148	1.00	16.81	AAAA
ATOM	1092	N	GLY	140	25.644	29.105	46.086	1.00	19.30	AAAA
ATOM	1093	CA	GLY	140	25.330	30.295	46.864	1.00	21.34	AAAA
ATOM	1094	C	GLY	140	26.393	31.378	46.888	1.00	20.19	AAAA
ATOM	1095	O	GLY	140	26.653	31.968	47.943	1.00	18.77	AAAA
ATOM	1096	N	PHE	141	26.996	31.649	45.733	1.00	15.52	AAAA
ATOM	1097	CA	PHE	141	28.034	32.675	45.600	1.00	20.71	AAAA
ATOM	1098	CB	PHE	141	27.711	33.952	46.388	1.00	20.03	AAAA
ATOM	1099	CG	PHE	141	26.355	34.544	46.127	1.00	28.32	AAAA
ATOM	1100	CD1	PHE	141	25.855	35.526	46.997	1.00	24.25	AAAA
ATOM	1101	CD2	PHE	141	25.589	34.170	45.029	1.00	30.11	AAAA
ATOM	1102	CE1	PHE	141	24.628	36.116	46.775	1.00	25.94	AAAA
ATOM	1103	CE2	PHE	141	24.346	34.766	44.801	1.00	21.61	AAAA
ATOM	1104	CZ	PHE	141	23.870	35.741	45.677	1.00	24.41	AAAA
ATOM	1105	C	PHE	141	29.357	32.188	46.158	1.00	14.45	AAAA
ATOM	1106	O	PHE	141	30.336	32.914	46.111	1.00	16.39	AAAA
ATOM	1107	N	CYS	142	29.389	30.982	46.716	1.00	16.77	AAAA
ATOM	1108	CA	CYS	142	30.629	30.466	47.285	1.00	17.71	AAAA
ATOM	1109	CB	CYS	142	30.347	29.845	48.659	1.00	13.95	AAAA
ATOM	1110	SG	CYS	142	29.606	30.985	49.846	1.00	16.63	AAAA
ATOM	1111	C	CYS	142	31.313	29.421	46.401	1.00	18.09	AAAA
ATOM	1112	O	CYS	142	30.647	28.527	45.856	1.00	16.60	AAAA
ATOM	1113	N	TYR	143	32.639	29.539	46.272	1.00	12.50	AAAA
ATOM	1114	CA	TYR	143	33.429	28.603	45.478	1.00	15.32	AAAA
ATOM	1115	CB	TYR	143	34.333	29.322	44.473	1.00	13.07	AAAA
ATOM	1116	CG	TYR	143	33.614	30.338	43.612	1.00	15.80	AAAA
ATOM	1117	CD1	TYR	143	33.396	31.636	44.071	1.00	15.48	AAAA
ATOM	1118	CE1	TYR	143	32.740	32.589	43.270	1.00	11.99	AAAA
ATOM	1119	CD2	TYR	143	33.157	29.999	42.336	1.00	14.60	AAAA
ATOM	1120	CE2	TYR	143	32.501	30.935	41.532	1.00	10.74	AAAA
ATOM	1121	CZ	TYR	143	32.301	32.229	42.008	1.00	20.89	AAAA
ATOM	1122	OH	TYR	143	31.698	33.177	41.208	1.00	18.87	AAAA

ATOM	1123	C	TYR	143	34.310	27.723	46.358	1.00	17.35	AAAA
ATOM	1124	O	TYR	143	34.581	26.574	46.013	1.00	16.67	AAAA
ATOM	1125	N	ILE	144	34.763	28.262	47.489	1.00	14.93	AAAA
ATOM	1126	CA	ILE	144	35.599	27.500	48.408	1.00	14.17	AAAA
ATOM	1127	CB	ILE	144	37.018	28.069	48.440	1.00	14.87	AAAA
ATOM	1128	CG2	ILE	144	37.864	27.332	49.474	1.00	13.55	AAAA
ATOM	1129	CG1	ILE	144	37.611	28.027	47.021	1.00	16.98	AAAA
ATOM	1130	CD1	ILE	144	39.052	28.537	46.901	1.00	17.42	AAAA
ATOM	1131	C	ILE	144	34.959	27.615	49.788	1.00	17.22	AAAA
ATOM	1132	O	ILE	144	34.606	28.716	50.220	1.00	14.72	AAAA
ATOM	1133	N	ASN	145	34.798	26.486	50.474	1.00	13.46	AAAA
ATOM	1134	CA	ASN	145	34.170	26.493	51.797	1.00	16.09	AAAA
ATOM	1135	CB	ASN	145	33.401	25.178	51.988	1.00	14.50	AAAA
ATOM	1136	CG	ASN	145	32.428	25.239	53.148	1.00	15.64	AAAA
ATOM	1137	OD1	ASN	145	32.800	25.587	54.263	1.00	14.97	AAAA
ATOM	1138	ND2	ASN	145	31.170	24.916	52.882	1.00	16.74	AAAA
ATOM	1139	C	ASN	145	35.266	26.639	52.873	1.00	15.04	AAAA
ATOM	1140	O	ASN	145	35.812	25.637	53.338	1.00	15.72	AAAA
ATOM	1141	N	ASN	146	35.599	27.865	53.282	1.00	12.34	AAAA
ATOM	1142	CA	ASN	146	36.685	28.006	54.262	1.00	15.31	AAAA
ATOM	1143	CB	ASN	146	37.161	29.464	54.354	1.00	15.81	AAAA
ATOM	1144	CG	ASN	146	36.101	30.396	54.865	1.00	15.25	AAAA
ATOM	1145	OD1	ASN	146	36.113	30.757	56.034	1.00	13.57	AAAA
ATOM	1146	ND2	ASN	146	35.156	30.775	53.996	1.00	10.85	AAAA
ATOM	1147	C	ASN	146	36.306	27.400	55.613	1.00	13.04	AAAA
ATOM	1148	O	ASN	146	37.160	26.865	56.314	1.00	14.76	AAAA
ATOM	1149	N	PRO	147	35.025	27.489	56.016	1.00	14.28	AAAA
ATOM	1150	CD	PRO	147	33.817	28.175	55.515	1.00	7.62	AAAA
ATOM	1151	CA	PRO	147	34.750	26.843	57.307	1.00	13.51	AAAA
ATOM	1152	CB	PRO	147	33.251	27.058	57.482	1.00	14.44	AAAA
ATOM	1153	CG	PRO	147	33.056	28.436	56.827	1.00	12.32	AAAA
ATOM	1154	C	PRO	147	35.118	25.330	57.278	1.00	18.86	AAAA
ATOM	1155	O	PRO	147	35.678	24.796	58.251	1.00	16.24	AAAA
ATOM	1156	N	ALA	148	34.818	24.642	56.171	1.00	15.01	AAAA
ATOM	1157	CA	ALA	148	35.122	23.200	56.080	1.00	15.58	AAAA
ATOM	1158	CB	ALA	148	34.402	22.561	54.882	1.00	12.93	AAAA
ATOM	1159	C	ALA	148	36.624	22.956	55.984	1.00	14.94	AAAA
ATOM	1160	O	ALA	148	37.138	21.999	56.560	1.00	14.69	AAAA
ATOM	1161	N	VAL	149	37.328	23.817	55.263	1.00	12.49	AAAA
ATOM	1162	CA	VAL	149	38.778	23.708	55.163	1.00	15.31	AAAA
ATOM	1163	CB	VAL	149	39.364	24.797	54.243	1.00	14.77	AAAA
ATOM	1164	CG1	VAL	149	40.899	24.870	54.369	1.00	14.68	AAAA
ATOM	1165	CG2	VAL	149	38.981	24.501	52.808	1.00	12.50	AAAA
ATOM	1166	C	VAL	149	39.323	23.887	56.572	1.00	20.14	AAAA
ATOM	1167	O	VAL	149	40.172	23.109	57.028	1.00	17.32	AAAA
ATOM	1168	N	GLY	150	38.815	24.899	57.271	1.00	15.45	AAAA
ATOM	1169	CA	GLY	150	39.284	25.168	58.622	1.00	20.96	AAAA
ATOM	1170	C	GLY	150	39.030	24.053	59.621	1.00	24.16	AAAA
ATOM	1171	O	GLY	150	39.888	23.738	60.458	1.00	19.50	AAAA
ATOM	1172	N	ILE	151	37.842	23.465	59.557	1.00	16.67	AAAA
ATOM	1173	CA	ILE	151	37.490	22.375	60.461	1.00	19.56	AAAA
ATOM	1174	CB	ILE	151	35.992	22.052	60.348	1.00	16.46	AAAA
ATOM	1175	CG2	ILE	151	35.667	20.709	61.036	1.00	17.93	AAAA
ATOM	1176	CG1	ILE	151	35.180	23.209	60.959	1.00	12.31	AAAA
ATOM	1177	CD1	ILE	151	33.686	23.123	60.672	1.00	18.71	AAAA
ATOM	1178	C	ILE	151	38.352	21.148	60.164	1.00	22.66	AAAA
ATOM	1179	O	ILE	151	38.796	20.472	61.087	1.00	20.08	AAAA
ATOM	1180	N	GLU	152	38.599	20.861	58.888	1.00	19.71	AAAA
ATOM	1181	CA	GLU	152	39.434	19.718	58.533	1.00	13.85	AAAA
ATOM	1182	CB	GLU	152	39.362	19.437	57.033	1.00	20.21	AAAA
ATOM	1183	CG	GLU	152	38.033	18.833	56.624	1.00	22.16	AAAA
ATOM	1184	CD	GLU	152	37.838	17.430	57.166	1.00	26.94	AAAA
ATOM	1185	OE1	GLU	152	36.720	16.906	57.035	1.00	25.03	AAAA
ATOM	1186	OE2	GLU	152	38.800	16.846	57.708	1.00	24.95	AAAA
ATOM	1187	C	GLU	152	40.865	20.010	58.942	1.00	16.85	AAAA
ATOM	1188	O	GLU	152	41.629	19.110	59.289	1.00	19.25	AAAA

ATOM	1189	N	TYR	153	41.228	21.290	58.931	1.00	14.74	AAAA
ATOM	1190	CA	TYR	153	42.574	21.672	59.350	1.00	17.71	AAAA
ATOM	1191	CB	TYR	153	42.757	23.193	59.179	1.00	13.26	AAAA
ATOM	1192	CG	TYR	153	44.059	23.727	59.729	1.00	16.36	AAAA
ATOM	1193	CD1	TYR	153	45.234	23.726	58.967	1.00	18.41	AAAA
ATOM	1194	CE1	TYR	153	46.438	24.219	59.511	1.00	21.03	AAAA
ATOM	1195	CD2	TYR	153	44.115	24.220	61.028	1.00	21.16	AAAA
ATOM	1196	CE2	TYR	153	45.288	24.705	61.570	1.00	19.76	AAAA
ATOM	1197	CZ	TYR	153	46.440	24.711	60.824	1.00	25.97	AAAA
ATOM	1198	OH	TYR	153	47.571	25.235	61.410	1.00	23.15	AAAA
ATOM	1199	C	TYR	153	42.712	21.274	60.828	1.00	20.00	AAAA
ATOM	1200	O	TYR	153	43.722	20.698	61.247	1.00	19.61	AAAA
ATOM	1201	N	LEU	154	41.683	21.569	61.616	1.00	17.78	AAAA
ATOM	1202	CA	LEU	154	41.698	21.239	63.042	1.00	17.26	AAAA
ATOM	1203	CB	LEU	154	40.511	21.913	63.744	1.00	20.44	AAAA
ATOM	1204	CG	LEU	154	40.636	23.434	63.942	1.00	19.57	AAAA
ATOM	1205	CD1	LEU	154	39.277	24.046	64.309	1.00	22.48	AAAA
ATOM	1206	CD2	LEU	154	41.692	23.709	65.044	1.00	20.84	AAAA
ATOM	1207	C	LEU	154	41.669	19.715	63.262	1.00	19.69	AAAA
ATOM	1208	O	LEU	154	42.357	19.191	64.149	1.00	22.91	AAAA
ATOM	1209	N	ARG	155	40.878	18.996	62.469	1.00	20.88	AAAA
ATOM	1210	CA	ARG	155	40.840	17.539	62.622	1.00	22.64	AAAA
ATOM	1211	CB	ARG	155	39.829	16.905	61.652	1.00	25.69	AAAA
ATOM	1212	CG	ARG	155	38.384	17.394	61.893	1.00	27.64	AAAA
ATOM	1213	CD	ARG	155	37.382	16.834	60.892	1.00	25.67	AAAA
ATOM	1214	NE	ARG	155	36.931	15.497	61.246	1.00	30.88	AAAA
ATOM	1215	CZ	ARG	155	36.135	14.753	60.488	1.00	36.28	AAAA
ATOM	1216	NH1	ARG	155	35.705	15.218	59.318	1.00	26.96	AAAA
ATOM	1217	NH2	ARG	155	35.737	13.562	60.923	1.00	27.33	AAAA
ATOM	1218	C	ARG	155	42.235	16.966	62.390	1.00	28.00	AAAA
ATOM	1219	O	ARG	155	42.674	16.070	63.119	1.00	28.05	AAAA
ATOM	1220	N	LYS	156	42.949	17.486	61.395	1.00	23.53	AAAA
ATOM	1221	CA	LYS	156	44.290	16.977	61.128	1.00	26.79	AAAA
ATOM	1222	CB	LYS	156	44.854	17.558	59.824	1.00	26.01	AAAA
ATOM	1223	CG	LYS	156	46.213	16.955	59.444	1.00	29.70	AAAA
ATOM	1224	CD	LYS	156	46.632	17.308	58.035	1.00	28.77	AAAA
ATOM	1225	CE	LYS	156	45.685	16.692	57.005	1.00	39.79	AAAA
ATOM	1226	NZ	LYS	156	45.671	15.192	57.058	1.00	36.33	AAAA
ATOM	1227	C	LYS	156	45.233	17.260	62.299	1.00	26.40	AAAA
ATOM	1228	O	LYS	156	46.188	16.511	62.529	1.00	26.19	AAAA
ATOM	1229	N	LYS	157	44.960	18.337	63.032	1.00	22.50	AAAA
ATOM	1230	CA	LYS	157	45.757	18.709	64.204	1.00	21.12	AAAA
ATOM	1231	CB	LYS	157	45.535	20.181	64.591	1.00	28.95	AAAA
ATOM	1232	CG	LYS	157	46.160	21.215	63.652	1.00	25.94	AAAA
ATOM	1233	CD	LYS	157	47.669	21.067	63.575	1.00	35.16	AAAA
ATOM	1234	CE	LYS	157	48.281	22.099	62.627	1.00	39.24	AAAA
ATOM	1235	NZ	LYS	157	49.742	21.869	62.406	1.00	40.01	AAAA
ATOM	1236	C	LYS	157	45.421	17.825	65.411	1.00	22.98	AAAA
ATOM	1237	O	LYS	157	46.085	17.903	66.444	1.00	27.77	AAAA
ATOM	1238	N	GLY	158	44.392	16.995	65.284	1.00	26.49	AAAA
ATOM	1239	CA	GLY	158	44.023	16.106	66.376	1.00	24.82	AAAA
ATOM	1240	C	GLY	158	42.771	16.459	67.161	1.00	33.13	AAAA
ATOM	1241	O	GLY	158	42.421	15.775	68.128	1.00	27.21	AAAA
ATOM	1242	N	PHE	159	42.085	17.529	66.781	1.00	27.47	AAAA
ATOM	1243	CA	PHE	159	40.866	17.861	67.502	1.00	24.15	AAAA
ATOM	1244	CB	PHE	159	40.410	19.285	67.186	1.00	27.53	AAAA
ATOM	1245	CG	PHE	159	41.264	20.343	67.827	1.00	27.26	AAAA
ATOM	1246	CD1	PHE	159	42.439	20.785	67.220	1.00	28.12	AAAA
ATOM	1247	CD2	PHE	159	40.926	20.842	69.076	1.00	21.10	AAAA
ATOM	1248	CE1	PHE	159	43.264	21.714	67.866	1.00	26.24	AAAA
ATOM	1249	CE2	PHE	159	41.738	21.768	69.736	1.00	26.07	AAAA
ATOM	1250	CZ	PHE	159	42.907	22.205	69.135	1.00	23.91	AAAA
ATOM	1251	C	PHE	159	39.792	16.854	67.120	1.00	29.02	AAAA
ATOM	1252	O	PHE	159	39.639	16.533	65.947	1.00	21.14	AAAA
ATOM	1253	N	LYS	160	39.056	16.361	68.110	1.00	24.79	AAAA
ATOM	1254	CA	LYS	160	38.011	15.366	67.881	1.00	24.26	AAAA

ATOM	1255	CB	LYS	160	38.360	14.098	68.668	1.00	22.86	AAAA
ATOM	1256	CG	LYS	160	39.625	13.424	68.157	1.00	43.16	AAAA
ATOM	1257	CD	LYS	160	40.222	12.417	69.141	1.00	54.05	AAAA
ATOM	1258	CE	LYS	160	39.236	11.343	69.577	1.00	62.87	AAAA
ATOM	1259	NZ	LYS	160	38.154	11.890	70.446	1.00	68.11	AAAA
ATOM	1260	C	LYS	160	36.599	15.822	68.225	1.00	21.12	AAAA
ATOM	1261	O	LYS	160	35.632	15.072	68.051	1.00	22.43	AAAA
ATOM	1262	N	ARG	161	36.476	17.042	68.733	1.00	19.68	AAAA
ATOM	1263	CA	ARG	161	35.164	17.594	69.073	1.00	20.84	AAAA
ATOM	1264	CB	ARG	161	34.865	17.467	70.572	1.00	26.02	AAAA
ATOM	1265	CG	ARG	161	34.715	16.031	71.080	1.00	28.47	AAAA
ATOM	1266	CD	ARG	161	34.213	16.025	72.523	1.00	30.38	AAAA
ATOM	1267	NE	ARG	161	35.098	16.734	73.445	1.00	32.99	AAAA
ATOM	1268	CZ	ARG	161	36.272	16.278	73.883	1.00	40.49	AAAA
ATOM	1269	NH1	ARG	161	36.724	15.094	73.489	1.00	31.49	AAAA
ATOM	1270	NH2	ARG	161	37.003	17.014	74.712	1.00	38.54	AAAA
ATOM	1271	C	ARG	161	35.171	19.060	68.680	1.00	18.98	AAAA
ATOM	1272	O	ARG	161	35.552	19.932	69.460	1.00	23.57	AAAA
ATOM	1273	N	ILE	162	34.743	19.332	67.458	1.00	19.82	AAAA
ATOM	1274	CA	ILE	162	34.744	20.700	66.947	1.00	17.81	AAAA
ATOM	1275	CB	ILE	162	35.522	20.717	65.626	1.00	18.33	AAAA
ATOM	1276	CG2	ILE	162	35.542	22.110	65.042	1.00	13.65	AAAA
ATOM	1277	CG1	ILE	162	36.937	20.200	65.895	1.00	18.15	AAAA
ATOM	1278	CD1	ILE	162	37.722	19.852	64.670	1.00	22.52	AAAA
ATOM	1279	C	ILE	162	33.316	21.184	66.724	1.00	14.71	AAAA
ATOM	1280	O	ILE	162	32.520	20.492	66.126	1.00	17.99	AAAA
ATOM	1281	N	LEU	163	32.996	22.374	67.217	1.00	16.93	AAAA
ATOM	1282	CA	LEU	163	31.653	22.902	67.061	1.00	20.73	AAAA
ATOM	1283	CB	LEU	163	31.115	23.376	68.421	1.00	18.45	AAAA
ATOM	1284	CG	LEU	163	29.846	24.236	68.463	1.00	19.99	AAAA
ATOM	1285	CD1	LEU	163	28.657	23.408	67.975	1.00	15.66	AAAA
ATOM	1286	CD2	LEU	163	29.609	24.751	69.870	1.00	18.74	AAAA
ATOM	1287	C	LEU	163	31.705	24.071	66.106	1.00	18.40	AAAA
ATOM	1288	O	LEU	163	32.607	24.889	66.188	1.00	18.65	AAAA
ATOM	1289	N	TYR	164	30.752	24.128	65.186	1.00	16.97	AAAA
ATOM	1290	CA	TYR	164	30.656	25.246	64.252	1.00	11.76	AAAA
ATOM	1291	CB	TYR	164	30.782	24.754	62.816	1.00	14.07	AAAA
ATOM	1292	CG	TYR	164	30.593	25.851	61.797	1.00	14.51	AAAA
ATOM	1293	CD1	TYR	164	31.573	26.822	61.562	1.00	27.08	AAAA
ATOM	1294	CE1	TYR	164	31.353	27.832	60.598	1.00	26.21	AAAA
ATOM	1295	CD2	TYR	164	29.415	25.916	61.070	1.00	21.45	AAAA
ATOM	1296	CE2	TYR	164	29.193	26.891	60.137	1.00	21.89	AAAA
ATOM	1297	CZ	TYR	164	30.148	27.839	59.896	1.00	16.35	AAAA
ATOM	1298	OH	TYR	164	29.857	28.764	58.913	1.00	27.44	AAAA
ATOM	1299	C	TYR	164	29.279	25.873	64.463	1.00	15.67	AAAA
ATOM	1300	O	TYR	164	28.760	25.177	64.455	1.00	16.07	AAAA
ATOM	1301	N	ILE	165	29.440	27.187	64.674	1.00	14.52	AAAA
ATOM	1302	CA	ILE	165	27.778	27.987	64.893	1.00	18.37	AAAA
ATOM	1303	CB	ILE	165	27.959	28.596	66.254	1.00	13.31	AAAA
ATOM	1304	CG2	ILE	165	26.654	29.359	66.419	1.00	13.06	AAAA
ATOM	1305	CG1	ILE	165	28.172	27.573	67.376	1.00	17.28	AAAA
ATOM	1306	CD1	ILE	165	28.493	28.209	68.739	1.00	15.02	AAAA
ATOM	1307	C	ILE	165	27.853	28.926	63.779	1.00	20.75	AAAA
ATOM	1308	O	ILE	165	28.759	29.733	63.569	1.00	16.67	AAAA
ATOM	1309	N	ASP	166	26.725	28.901	63.084	1.00	15.37	AAAA
ATOM	1310	CA	ASP	166	26.503	29.779	61.942	1.00	15.63	AAAA
ATOM	1311	CB	ASP	166	26.276	28.885	60.698	1.00	12.31	AAAA
ATOM	1312	CG	ASP	166	26.279	29.666	59.393	1.00	16.37	AAAA
ATOM	1313	OD1	ASP	166	25.378	30.508	59.213	1.00	13.41	AAAA
ATOM	1314	OD2	ASP	166	27.187	29.428	58.551	1.00	16.06	AAAA
ATOM	1315	C	ASP	166	25.334	30.740	62.174	1.00	15.54	AAAA
ATOM	1316	O	ASP	166	24.160	30.355	62.137	1.00	12.60	AAAA
ATOM	1317	N	LEU	167	25.647	32.010	62.407	1.00	14.02	AAAA
ATOM	1318	CA	LEU	167	24.598	32.993	62.665	1.00	12.05	AAAA
ATOM	1319	CB	LEU	167	25.051	33.962	63.767	1.00	14.61	AAAA
ATOM	1320	CG	LEU	167	25.345	33.239	65.091	1.00	17.20	AAAA

ATOM	1321	CD1	LEU	167	25.635	34.271	66.169	1.00	28.82	AAAA
ATOM	1322	CD2	LEU	167	24.148	32.372	65.513	1.00	18.59	AAAA
ATOM	1323	C	LEU	167	24.122	33.776	61.449	1.00	12.62	AAAA
ATOM	1324	O	LEU	167	23.288	34.678	61.570	1.00	15.00	AAAA
ATOM	1325	N	ASP	168	24.667	33.431	60.288	1.00	14.35	AAAA
ATOM	1326	CA	ASP	168	24.277	34.056	59.022	1.00	19.50	AAAA
ATOM	1327	CB	ASP	168	25.060	33.409	57.880	1.00	25.15	AAAA
ATOM	1328	CG	ASP	168	24.908	34.145	56.573	1.00	48.45	AAAA
ATOM	1329	OD1	ASP	168	25.477	35.247	56.454	1.00	64.45	AAAA
ATOM	1330	OD2	ASP	168	24.215	33.633	55.668	1.00	44.71	AAAA
ATOM	1331	C	ASP	168	22.787	33.751	58.834	1.00	16.30	AAAA
ATOM	1332	O	ASP	168	22.327	32.696	59.252	1.00	17.72	AAAA
ATOM	1333	N	ALA	169	22.059	34.657	58.175	1.00	14.11	AAAA
ATOM	1334	CA	ALA	169	20.618	34.503	57.934	1.00	19.61	AAAA
ATOM	1335	CB	ALA	169	20.006	35.856	57.470	1.00	13.56	AAAA
ATOM	1336	C	ALA	169	20.277	33.400	56.926	1.00	18.23	AAAA
ATOM	1337	O	ALA	169	19.105	33.159	56.641	1.00	17.20	AAAA
ATOM	1338	N	HIS	170	21.301	32.750	56.373	1.00	16.53	AAAA
ATOM	1339	CA	HIS	170	21.075	31.652	55.436	1.00	17.51	AAAA
ATOM	1340	CB	HIS	170	21.616	31.973	54.033	1.00	22.32	AAAA
ATOM	1341	CG	HIS	170	20.954	33.142	53.377	1.00	25.38	AAAA
ATOM	1342	CD2	HIS	170	19.934	33.196	52.487	1.00	19.33	AAAA
ATOM	1343	ND1	HIS	170	21.308	34.448	53.638	1.00	18.17	AAAA
ATOM	1344	CE1	HIS	170	20.535	35.257	52.935	1.00	30.34	AAAA
ATOM	1345	NE2	HIS	170	19.692	34.523	52.229	1.00	17.51	AAAA
ATOM	1346	C	HIS	170	21.781	30.413	55.967	1.00	16.72	AAAA
ATOM	1347	O	HIS	170	22.827	30.511	56.610	1.00	15.92	AAAA
ATOM	1348	N	HIS	171	21.209	29.245	55.682	1.00	15.28	AAAA
ATOM	1349	CA	HIS	171	21.751	27.961	56.123	1.00	12.53	AAAA
ATOM	1350	CB	HIS	171	20.702	26.878	55.814	1.00	14.09	AAAA
ATOM	1351	CG	HIS	171	21.180	25.468	55.980	1.00	17.27	AAAA
ATOM	1352	CD2	HIS	171	21.249	24.447	55.090	1.00	12.48	AAAA
ATOM	1353	ND1	HIS	171	21.622	24.956	57.181	1.00	26.73	AAAA
ATOM	1354	CE1	HIS	171	21.948	23.685	57.021	1.00	15.98	AAAA
ATOM	1355	NE2	HIS	171	21.729	23.352	55.761	1.00	20.03	AAAA
ATOM	1356	C	HIS	171	23.107	27.602	55.498	1.00	15.55	AAAA
ATOM	1357	O	HIS	171	23.318	27.784	54.298	1.00	17.03	AAAA
ATOM	1358	N	CYS	172	24.026	27.105	56.323	1.00	14.33	AAAA
ATOM	1359	CA	CYS	172	25.350	26.675	55.866	1.00	13.65	AAAA
ATOM	1360	CB	CYS	172	26.330	26.631	57.054	1.00	12.99	AAAA
ATOM	1361	SG	CYS	172	25.680	25.826	58.551	1.00	17.17	AAAA
ATOM	1362	C	CYS	172	25.212	25.274	55.257	1.00	16.52	AAAA
ATOM	1363	O	CYS	172	25.750	24.297	55.783	1.00	14.95	AAAA
ATOM	1364	N	ASP	173	24.516	25.173	54.130	1.00	15.42	AAAA
ATOM	1365	CA	ASP	173	24.302	23.865	53.531	1.00	14.75	AAAA
ATOM	1366	CB	ASP	173	23.339	23.956	52.332	1.00	17.73	AAAA
ATOM	1367	CG	ASP	173	23.765	24.966	51.283	1.00	22.84	AAAA
ATOM	1368	OD1	ASP	173	23.106	24.998	50.216	1.00	18.68	AAAA
ATOM	1369	OD2	ASP	173	24.730	25.728	51.504	1.00	15.34	AAAA
ATOM	1370	C	ASP	173	25.590	23.145	53.149	1.00	16.39	AAAA
ATOM	1371	O	ASP	173	25.684	21.922	53.279	1.00	16.48	AAAA
ATOM	1372	N	GLY	174	26.583	23.912	52.705	1.00	15.58	AAAA
ATOM	1373	CA	GLY	174	27.869	23.346	52.360	1.00	13.97	AAAA
ATOM	1374	C	GLY	174	28.508	22.723	53.595	1.00	18.44	AAAA
ATOM	1375	O	GLY	174	28.970	21.586	53.540	1.00	15.48	AAAA
ATOM	1376	N	VAL	175	28.554	23.456	54.706	1.00	16.84	AAAA
ATOM	1377	CA	VAL	175	29.136	22.923	55.946	1.00	16.54	AAAA
ATOM	1378	CB	VAL	175	29.201	24.031	57.037	1.00	15.88	AAAA
ATOM	1379	CG1	VAL	175	29.927	23.507	58.307	1.00	15.35	AAAA
ATOM	1380	CG2	VAL	175	29.923	25.258	56.476	1.00	15.62	AAAA
ATOM	1381	C	VAL	175	28.318	21.720	56.467	1.00	19.21	AAAA
ATOM	1382	O	VAL	175	28.876	20.735	56.961	1.00	17.75	AAAA
ATOM	1383	N	GLN	176	26.996	21.798	56.367	1.00	17.74	AAAA
ATOM	1384	CA	GLN	176	26.164	20.685	56.832	1.00	15.66	AAAA
ATOM	1385	CB	GLN	176	24.678	20.973	56.595	1.00	16.64	AAAA
ATOM	1386	CG	GLN	176	23.789	19.788	56.952	1.00	17.00	AAAA

Figure 16-22

ATOM	1387	CD	GLN	176	22.325	20.106	56.884	1.00	21.52	AAAA
ATOM	1388	OE1	GLN	176	21.850	21.016	57.567	1.00	21.72	AAAA
ATOM	1389	NE2	GLN	176	21.581	19.348	56.064	1.00	20.30	AAAA
ATOM	1390	C	GLN	176	26.527	19.387	56.121	1.00	16.33	AAAA
ATOM	1391	O	GLN	176	26.751	18.354	56.748	1.00	17.46	AAAA
ATOM	1392	N	GLU	177	26.581	19.443	54.799	1.00	22.24	AAAA
ATOM	1393	CA	GLU	177	26.909	18.251	54.021	1.00	19.67	AAAA
ATOM	1394	CB	GLU	177	26.857	18.587	52.533	1.00	15.55	AAAA
ATOM	1395	CG	GLU	177	27.131	17.388	51.623	1.00	20.24	AAAA
ATOM	1396	CD	GLU	177	26.960	17.740	50.159	1.00	27.00	AAAA
ATOM	1397	OE1	GLU	177	27.974	17.935	49.450	1.00	30.23	AAAA
ATOM	1398	OE2	GLU	177	25.796	17.853	49.725	1.00	26.89	AAAA
ATOM	1399	C	GLU	177	28.284	17.713	54.376	1.00	20.42	AAAA
ATOM	1400	O	GLU	177	28.486	16.503	54.527	1.00	17.05	AAAA
ATOM	1401	N	ALA	178	29.233	18.626	54.527	1.00	19.67	AAAA
ATOM	1402	CA	ALA	178	30.611	18.259	54.839	1.00	18.18	AAAA
ATOM	1403	CB	ALA	178	31.464	19.519	54.918	1.00	12.76	AAAA
ATOM	1404	C	ALA	178	30.806	17.418	56.106	1.00	17.56	AAAA
ATOM	1405	O	ALA	178	31.690	16.555	56.167	1.00	17.72	AAAA
ATOM	1406	N	PHE	179	29.981	17.656	57.116	1.00	18.82	AAAA
ATOM	1407	CA	PHE	179	30.124	16.945	58.379	1.00	20.26	AAAA
ATOM	1408	CB	PHE	179	30.554	17.948	59.439	1.00	13.17	AAAA
ATOM	1409	CG	PHE	179	31.779	18.693	59.048	1.00	16.28	AAAA
ATOM	1410	CD1	PHE	179	31.705	20.017	58.610	1.00	13.77	AAAA
ATOM	1411	CD2	PHE	179	33.002	18.031	58.995	1.00	15.57	AAAA
ATOM	1412	CE1	PHE	179	32.845	20.673	58.114	1.00	20.03	AAAA
ATOM	1413	CE2	PHE	179	34.145	18.677	58.500	1.00	20.30	AAAA
ATOM	1414	CZ	PHE	179	34.060	20.002	58.058	1.00	19.51	AAAA
ATOM	1415	C	PHE	179	28.882	16.219	58.833	1.00	18.52	AAAA
ATOM	1416	O	PHE	179	28.773	15.828	60.000	1.00	20.21	AAAA
ATOM	1417	N	TYR	180	27.969	16.016	57.895	1.00	18.33	AAAA
ATOM	1418	CA	TYR	180	26.698	15.379	58.176	1.00	19.93	AAAA
ATOM	1419	CB	TYR	180	25.874	15.310	56.894	1.00	20.97	AAAA
ATOM	1420	CG	TYR	180	24.402	15.341	57.159	1.00	19.80	AAAA
ATOM	1421	CD1	TYR	180	23.565	14.337	56.686	1.00	23.87	AAAA
ATOM	1422	CE1	TYR	180	22.203	14.391	56.898	1.00	21.32	AAAA
ATOM	1423	CD2	TYR	180	23.831	16.416	57.865	1.00	19.02	AAAA
ATOM	1424	CE2	TYR	180	22.470	16.482	58.084	1.00	26.84	AAAA
ATOM	1425	CZ	TYR	180	21.659	15.462	57.594	1.00	30.54	AAAA
ATOM	1426	OH	TYR	180	20.310	15.514	57.794	1.00	22.81	AAAA
ATOM	1427	C	TYR	180	26.855	13.970	58.737	1.00	22.61	AAAA
ATOM	1428	O	TYR	180	26.064	13.526	59.579	1.00	23.44	AAAA
ATOM	1429	N	ASP	181	27.893	13.298	58.253	1.00	22.27	AAAA
ATOM	1430	CA	ASP	181	28.245	11.920	58.590	1.00	33.84	AAAA
ATOM	1431	CB	ASP	181	28.916	11.318	57.339	1.00	41.74	AAAA
ATOM	1432	CG	ASP	181	30.035	10.363	57.662	1.00	57.71	AAAA
ATOM	1433	OD1	ASP	181	30.999	10.780	58.340	1.00	61.40	AAAA
ATOM	1434	OD2	ASP	181	29.965	9.197	57.221	1.00	65.77	AAAA
ATOM	1435	C	ASP	181	29.107	11.654	59.838	1.00	30.21	AAAA
ATOM	1436	O	ASP	181	29.307	10.497	60.227	1.00	27.84	AAAA
ATOM	1437	N	THR	182	29.615	12.696	60.480	1.00	27.53	AAAA
ATOM	1438	CA	THR	182	30.472	12.466	61.634	1.00	21.19	AAAA
ATOM	1439	CB	THR	182	31.918	12.977	61.358	1.00	26.55	AAAA
ATOM	1440	OG1	THR	182	32.729	12.763	62.513	1.00	25.62	AAAA
ATOM	1441	CG2	THR	182	31.922	14.471	61.037	1.00	21.67	AAAA
ATOM	1442	C	THR	182	30.010	13.050	62.954	1.00	25.02	AAAA
ATOM	1443	O	THR	182	29.306	14.049	62.992	1.00	23.56	AAAA
ATOM	1444	N	ASP	183	30.434	12.424	64.042	1.00	19.66	AAAA
ATOM	1445	CA	ASP	183	30.086	12.894	65.371	1.00	21.52	AAAA
ATOM	1446	CB	ASP	183	29.735	11.700	66.275	1.00	28.52	AAAA
ATOM	1447	CG	ASP	183	30.920	10.783	66.523	1.00	32.30	AAAA
ATOM	1448	OD1	ASP	183	31.667	10.502	65.565	1.00	30.99	AAAA
ATOM	1449	OD2	ASP	183	31.095	10.326	67.675	1.00	48.65	AAAA
ATOM	1450	C	ASP	183	31.257	13.685	65.947	1.00	16.66	AAAA
ATOM	1451	O	ASP	183	31.236	14.092	67.104	1.00	23.37	AAAA
ATOM	1452	N	GLN	184	32.286	13.909	65.131	1.00	21.95	AAAA

Figure 16-23

ATOM	1453	CA	GLN	184	33.437	14.672	65.590	1.00	17.65	AAAA
ATOM	1454	CB	GLN	184	34.701	14.243	64.866	1.00	21.36	AAAA
ATOM	1455	CG	GLN	184	35.068	12.790	65.102	1.00	27.38	AAAA
ATOM	1456	CD	GLN	184	36.485	12.476	64.691	1.00	31.96	AAAA
ATOM	1457	OE1	GLN	184	36.899	12.760	63.573	1.00	29.90	AAAA
ATOM	1458	NE2	GLN	184	37.239	11.878	65.599	1.00	31.84	AAAA
ATOM	1459	C	GLN	184	33.207	16.165	65.382	1.00	18.54	AAAA
ATOM	1460	O	GLN	184	33.881	17.009	65.972	1.00	18.11	AAAA
ATOM	1461	N	VAL	185	32.258	16.481	64.519	1.00	19.18	AAAA
ATOM	1462	CA	VAL	185	31.934	17.872	64.267	1.00	21.57	AAAA
ATOM	1463	CB	VAL	185	32.261	18.264	62.807	1.00	22.64	AAAA
ATOM	1464	CG1	VAL	185	31.994	19.768	62.591	1.00	16.26	AAAA
ATOM	1465	CG2	VAL	185	33.722	17.924	62.500	1.00	16.77	AAAA
ATOM	1466	C	VAL	185	30.449	18.035	64.523	1.00	16.91	AAAA
ATOM	1467	O	VAL	185	29.658	17.156	64.179	1.00	20.79	AAAA
ATOM	1468	N	PHE	186	30.081	19.146	65.153	1.00	18.73	AAAA
ATOM	1469	CA	PHE	186	28.687	19.446	65.435	1.00	16.22	AAAA
ATOM	1470	CB	PHE	186	28.432	19.559	66.952	1.00	16.83	AAAA
ATOM	1471	CG	PHE	186	26.976	19.682	67.299	1.00	17.96	AAAA
ATOM	1472	CD1	PHE	186	26.319	18.656	67.968	1.00	23.24	AAAA
ATOM	1473	CD2	PHE	186	26.240	20.797	66.904	1.00	15.41	AAAA
ATOM	1474	CE1	PHE	186	24.953	18.738	68.235	1.00	18.99	AAAA
ATOM	1475	CE2	PHE	186	24.879	20.887	67.168	1.00	24.05	AAAA
ATOM	1476	CZ	PHE	186	24.234	19.846	67.838	1.00	22.93	AAAA
ATOM	1477	C	PHE	186	28.437	20.789	64.778	1.00	17.16	AAAA
ATOM	1478	O	PHE	186	29.192	21.725	64.993	1.00	19.37	AAAA
ATOM	1479	N	VAL	187	27.391	20.874	63.961	1.00	19.67	AAAA
ATOM	1480	CA	VAL	187	27.075	22.116	63.277	1.00	17.74	AAAA
ATOM	1481	CB	VAL	187	27.010	21.914	61.720	1.00	18.65	AAAA
ATOM	1482	CG1	VAL	187	26.578	23.211	61.024	1.00	17.31	AAAA
ATOM	1483	CG2	VAL	187	28.359	21.453	61.194	1.00	16.65	AAAA
ATOM	1484	C	VAL	187	25.732	22.637	63.746	1.00	18.46	AAAA
ATOM	1485	O	VAL	187	24.752	21.903	63.764	1.00	20.64	AAAA
ATOM	1486	N	LEU	188	25.708	23.899	64.150	1.00	14.42	AAAA
ATOM	1487	CA	LEU	188	24.482	24.563	64.567	1.00	16.68	AAAA
ATOM	1488	CB	LEU	188	24.568	25.070	66.009	1.00	13.98	AAAA
ATOM	1489	CG	LEU	188	23.522	26.119	66.450	1.00	13.66	AAAA
ATOM	1490	CD1	LEU	188	22.103	25.556	66.401	1.00	15.55	AAAA
ATOM	1491	CD2	LEU	188	23.844	26.585	67.861	1.00	16.40	AAAA
ATOM	1492	C	LEU	188	24.272	25.756	63.667	1.00	20.01	AAAA
ATOM	1493	O	LEU	188	25.164	26.595	63.506	1.00	18.86	AAAA
ATOM	1494	N	SER	189	23.106	25.845	63.057	1.00	14.46	AAAA
ATOM	1495	CA	SER	189	22.841	27.011	62.230	1.00	14.56	AAAA
ATOM	1496	CB	SER	189	22.896	26.668	60.737	1.00	15.55	AAAA
ATOM	1497	OG	SER	189	22.619	27.851	60.008	1.00	14.09	AAAA
ATOM	1498	C	SER	189	21.487	27.606	62.508	1.00	15.24	AAAA
ATOM	1499	O	SER	189	20.509	26.885	62.578	1.00	21.46	AAAA
ATOM	1500	N	LEU	190	21.423	28.921	62.690	1.00	14.92	AAAA
ATOM	1501	CA	LEU	190	20.128	29.572	62.826	1.00	15.54	AAAA
ATOM	1502	CB	LEU	190	20.084	30.663	63.906	1.00	21.02	AAAA
ATOM	1503	CG	LEU	190	20.594	30.532	65.339	1.00	30.17	AAAA
ATOM	1504	CD1	LEU	190	19.736	31.437	66.210	1.00	19.75	AAAA
ATOM	1505	CD2	LEU	190	20.547	29.130	65.831	1.00	19.08	AAAA
ATOM	1506	C	LEU	190	20.035	30.250	61.456	1.00	14.31	AAAA
ATOM	1507	O	LEU	190	21.031	30.752	60.951	1.00	15.43	AAAA
ATOM	1508	N	HIS	191	18.855	30.285	60.856	1.00	16.88	AAAA
ATOM	1509	CA	HIS	191	18.732	30.884	59.535	1.00	14.34	AAAA
ATOM	1510	CB	HIS	191	19.506	30.015	58.539	1.00	17.34	AAAA
ATOM	1511	CG	HIS	191	19.229	28.546	58.697	1.00	14.27	AAAA
ATOM	1512	CD2	HIS	191	19.941	27.578	59.319	1.00	9.60	AAAA
ATOM	1513	ND1	HIS	191	18.073	27.940	58.247	1.00	21.22	AAAA
ATOM	1514	CE1	HIS	191	18.088	26.660	58.582	1.00	17.22	AAAA
ATOM	1515	NE2	HIS	191	19.212	26.415	59.232	1.00	20.70	AAAA
ATOM	1516	C	HIS	191	17.277	31.026	59.110	1.00	16.19	AAAA
ATOM	1517	O	HIS	191	16.381	30.489	59.766	1.00	16.73	AAAA
ATOM	1518	N	GLN	192	17.044	31.796	58.045	1.00	14.78	AAAA

Figure 16-24

ATOM	1519	CA	GLN	192	15.683	31.968	57.516	1.00	16.33	AAAA
ATOM	1520	CB	GLN	192	15.669	32.871	56.283	1.00	17.07	AAAA
ATOM	1521	CG	GLN	192	16.174	34.270	56.498	1.00	18.15	AAAA
ATOM	1522	CD	GLN	192	16.408	34.965	55.177	1.00	14.74	AAAA
ATOM	1523	OE1	GLN	192	15.490	35.566	54.587	1.00	20.46	AAAA
ATOM	1524	NE2	GLN	192	17.630	34.839	54.665	1.00	13.44	AAAA
ATOM	1525	C	GLN	192	15.262	30.584	57.072	1.00	15.06	AAAA
ATOM	1526	O	GLN	192	16.071	29.843	56.514	1.00	19.23	AAAA
ATOM	1527	N	SER	193	14.007	30.223	57.304	1.00	15.63	AAAA
ATOM	1528	CA	SER	193	13.561	28.907	56.877	1.00	13.84	AAAA
ATOM	1529	CB	SER	193	12.097	28.677	57.284	1.00	17.28	AAAA
ATOM	1530	OG	SER	193	11.639	27.439	56.750	1.00	17.58	AAAA
ATOM	1531	C	SER	193	13.687	28.704	55.350	1.00	11.80	AAAA
ATOM	1532	O	SER	193	13.400	29.601	54.569	1.00	18.44	AAAA
ATOM	1533	N	PRO	194	14.103	27.505	54.928	1.00	14.59	AAAA
ATOM	1534	CD	PRO	194	14.335	26.325	55.782	1.00	19.22	AAAA
ATOM	1535	CA	PRO	194	14.268	27.143	53.513	1.00	15.30	AAAA
ATOM	1536	CB	PRO	194	14.892	25.737	53.573	1.00	18.33	AAAA
ATOM	1537	CG	PRO	194	15.359	25.587	55.007	1.00	22.34	AAAA
ATOM	1538	C	PRO	194	12.880	27.104	52.866	1.00	16.40	AAAA
ATOM	1539	O	PRO	194	12.757	27.003	51.640	1.00	19.43	AAAA
ATOM	1540	N	GLU	195	11.828	27.151	53.681	1.00	20.57	AAAA
ATOM	1541	CA	GLU	195	10.483	27.161	53.099	1.00	30.15	AAAA
ATOM	1542	CB	GLU	195	9.386	27.037	54.173	1.00	31.91	AAAA
ATOM	1543	CG	GLU	195	8.987	28.325	54.879	1.00	45.60	AAAA
ATOM	1544	CD	GLU	195	7.880	29.119	54.174	1.00	34.45	AAAA
ATOM	1545	OE1	GLU	195	7.635	30.259	54.612	1.00	43.98	AAAA
ATOM	1546	OE2	GLU	195	7.241	28.627	53.210	1.00	38.39	AAAA
ATOM	1547	C	GLU	195	10.333	28.474	52.318	1.00	26.92	AAAA
ATOM	1548	O	GLU	195	9.522	28.557	51.395	1.00	24.59	AAAA
ATOM	1549	N	TYR	196	11.116	29.501	52.669	1.00	18.16	AAAA
ATOM	1550	CA	TYR	196	11.024	30.753	51.922	1.00	15.81	AAAA
ATOM	1551	CB	TYR	196	10.208	31.801	52.690	1.00	20.01	AAAA
ATOM	1552	CG	TYR	196	10.868	32.353	53.932	1.00	19.77	AAAA
ATOM	1553	CD1	TYR	196	11.779	33.408	53.853	1.00	18.24	AAAA
ATOM	1554	CE1	TYR	196	12.407	33.898	54.988	1.00	18.50	AAAA
ATOM	1555	CD2	TYR	196	10.598	31.801	55.185	1.00	18.12	AAAA
ATOM	1556	CE2	TYR	196	11.223	32.283	56.339	1.00	21.09	AAAA
ATOM	1557	CZ	TYR	196	12.125	33.326	56.235	1.00	20.39	AAAA
ATOM	1558	OH	TYR	196	12.759	33.784	57.367	1.00	16.20	AAAA
ATOM	1559	C	TYR	196	12.342	31.372	51.475	1.00	16.89	AAAA
ATOM	1560	O	TYR	196	12.336	32.347	50.718	1.00	23.08	AAAA
ATOM	1561	N	ALA	197	13.466	30.817	51.911	1.00	17.52	AAAA
ATOM	1562	CA	ALA	197	14.754	31.400	51.512	1.00	20.26	AAAA
ATOM	1563	CB	ALA	197	15.315	32.261	52.659	1.00	20.74	AAAA
ATOM	1564	C	ALA	197	15.814	30.392	51.074	1.00	13.51	AAAA
ATOM	1565	O	ALA	197	15.787	29.229	51.457	1.00	19.35	AAAA
ATOM	1566	N	PHE	198	16.757	30.869	50.257	1.00	18.01	AAAA
ATOM	1567	CA	PHE	198	17.861	30.049	49.782	1.00	17.97	AAAA
ATOM	1568	CB	PHE	198	18.929	30.933	49.119	1.00	20.38	AAAA
ATOM	1569	CG	PHE	198	20.094	30.162	48.545	1.00	23.61	AAAA
ATOM	1570	CD1	PHE	198	20.039	29.660	47.245	1.00	29.71	AAAA
ATOM	1571	CD2	PHE	198	21.229	29.899	49.321	1.00	19.06	AAAA
ATOM	1572	CE1	PHE	198	21.091	28.908	46.719	1.00	30.39	AAAA
ATOM	1573	CE2	PHE	198	22.290	29.145	48.807	1.00	23.17	AAAA
ATOM	1574	CE	PHE	198	22.218	28.646	47.493	1.00	22.74	AAAA
ATOM	1575	C	PHE	198	18.453	29.419	51.032	1.00	16.02	AAAA
ATOM	1576	O	PHE	198	18.552	30.073	52.061	1.00	20.95	AAAA
ATOM	1577	N	PRO	199	18.941	28.176	50.937	1.00	19.92	AAAA
ATOM	1578	CD	PRO	199	19.600	27.508	52.074	1.00	17.86	AAAA
ATOM	1579	CA	PRO	199	18.990	27.318	49.744	1.00	23.54	AAAA
ATOM	1580	CB	PRO	199	20.108	26.344	50.095	1.00	22.70	AAAA
ATOM	1581	CG	PRO	199	19.813	26.087	51.534	1.00	23.16	AAAA
ATOM	1582	C	PRO	199	17.710	26.595	49.312	1.00	30.97	AAAA
ATOM	1583	O	PRO	199	17.733	25.855	48.322	1.00	23.25	AAAA
ATOM	1584	N	PHE	200	16.621	26.795	50.054	1.00	20.32	AAAA

43/263
Figure 16-25

ATOM	1585	CA	PHE	200	15.319	26.166	49.752	1.00	20.27	AAAA
ATOM	1586	CB	PHE	200	14.840	26.533	48.346	1.00	19.77	AAAA
ATOM	1587	CG	PHE	200	14.752	27.999	48.082	1.00	18.06	AAAA
ATOM	1588	CD1	PHE	200	15.742	28.644	47.346	1.00	18.97	AAAA
ATOM	1589	CD2	PHE	200	13.654	28.736	48.519	1.00	19.06	AAAA
ATOM	1590	CE1	PHE	200	15.635	30.003	47.042	1.00	21.67	AAAA
ATOM	1591	CE2	PHE	200	13.539	30.101	48.221	1.00	22.60	AAAA
ATOM	1592	CZ	PHE	200	14.527	30.736	47.482	1.00	18.93	AAAA
ATOM	1593	C	PHE	200	15.294	24.637	49.845	1.00	18.44	AAAA
ATOM	1594	O	PHE	200	14.302	24.049	50.272	1.00	20.74	AAAA
ATOM	1595	N	GLU	201	16.384	24.004	49.418	1.00	20.77	AAAA
ATOM	1596	CA	GLU	201	16.522	22.542	49.399	1.00	27.34	AAAA
ATOM	1597	CB	GLU	201	17.498	22.146	48.284	1.00	28.99	AAAA
ATOM	1598	CG	GLU	201	17.024	22.458	46.881	1.00	34.82	AAAA
ATOM	1599	CD	GLU	201	18.123	22.265	45.848	1.00	32.40	AAAA
ATOM	1600	OE1	GLU	201	18.701	21.155	45.769	1.00	38.28	AAAA
ATOM	1601	OE2	GLU	201	18.405	23.230	45.111	1.00	40.08	AAAA
ATOM	1602	C	GLU	201	17.007	21.891	50.695	1.00	23.51	AAAA
ATOM	1603	O	GLU	201	16.845	20.689	50.886	1.00	23.17	AAAA
ATOM	1604	N	LYS	202	17.619	22.681	51.571	1.00	20.03	AAAA
ATOM	1605	CA	LYS	202	18.178	22.177	52.829	1.00	17.01	AAAA
ATOM	1606	CB	LYS	202	19.666	21.862	52.634	1.00	19.24	AAAA
ATOM	1607	CG	LYS	202	19.903	20.769	51.611	1.00	36.04	AAAA
ATOM	1608	CD	LYS	202	20.997	21.162	50.648	1.00	45.11	AAAA
ATOM	1609	CE	LYS	202	21.060	20.209	49.463	1.00	55.83	AAAA
ATOM	1610	NZ	LYS	202	22.024	20.662	48.422	1.00	28.09	AAAA
ATOM	1611	C	LYS	202	18.016	23.240	53.899	1.00	17.02	AAAA
ATOM	1612	O	LYS	202	17.705	24.381	53.585	1.00	20.20	AAAA
ATOM	1613	N	GLY	203	18.232	22.875	55.160	1.00	22.94	AAAA
ATOM	1614	CA	GLY	203	18.064	23.850	56.223	1.00	19.38	AAAA
ATOM	1615	C	GLY	203	16.874	23.564	57.128	1.00	20.48	AAAA
ATOM	1616	O	GLY	203	16.607	24.312	58.070	1.00	18.55	AAAA
ATOM	1617	N	PHE	204	16.150	22.484	56.852	1.00	15.42	AAAA
ATOM	1618	CA	PHE	204	14.983	22.143	57.670	1.00	20.73	AAAA
ATOM	1619	CB	PHE	204	14.018	21.212	56.903	1.00	19.97	AAAA
ATOM	1620	CG	PHE	204	13.441	21.838	55.667	1.00	19.63	AAAA
ATOM	1621	CD1	PHE	204	14.137	21.801	54.459	1.00	24.96	AAAA
ATOM	1622	CD2	PHE	204	12.230	22.523	55.725	1.00	18.92	AAAA
ATOM	1623	CE1	PHE	204	13.636	22.438	53.327	1.00	20.66	AAAA
ATOM	1624	CE2	PHE	204	11.720	23.169	54.597	1.00	24.86	AAAA
ATOM	1625	CZ	PHE	204	12.422	23.127	53.400	1.00	23.66	AAAA
ATOM	1626	C	PHE	204	15.376	21.513	59.006	1.00	18.73	AAAA
ATOM	1627	O	PHE	204	16.415	20.851	59.131	1.00	20.18	AAAA
ATOM	1628	N	LEU	205	14.518	21.726	59.994	1.00	19.46	AAAA
ATOM	1629	CA	LEU	205	14.727	21.244	61.356	1.00	21.09	AAAA
ATOM	1630	CB	LEU	205	13.547	21.674	62.233	1.00	23.44	AAAA
ATOM	1631	CG	LEU	205	13.506	21.222	63.693	1.00	23.23	AAAA
ATOM	1632	CD1	LEU	205	14.717	21.736	64.445	1.00	24.06	AAAA
ATOM	1633	CD2	LEU	205	12.224	21.743	64.312	1.00	30.63	AAAA
ATOM	1634	C	LEU	205	14.943	19.748	61.489	1.00	23.53	AAAA
ATOM	1635	O	LEU	205	15.659	19.315	62.381	1.00	21.28	AAAA
ATOM	1636	N	GLU	206	14.356	18.959	60.591	1.00	21.59	AAAA
ATOM	1637	CA	GLU	206	14.487	17.502	60.686	1.00	27.89	AAAA
ATOM	1638	CB	GLU	206	13.345	16.816	59.928	1.00	28.90	AAAA
ATOM	1639	CG	GLU	206	12.060	17.615	59.942	1.00	48.55	AAAA
ATOM	1640	CD	GLU	206	12.169	18.832	59.042	1.00	46.86	AAAA
ATOM	1641	OE1	GLU	206	11.360	19.769	59.178	1.00	21.58	AAAA
ATOM	1642	OE2	GLU	206	13.076	18.833	58.181	1.00	63.58	AAAA
ATOM	1643	C	GLU	206	15.819	16.955	60.188	1.00	22.86	AAAA
ATOM	1644	O	GLU	206	16.071	15.753	60.286	1.00	21.21	AAAA
ATOM	1645	N	GLU	207	16.666	17.816	59.631	1.00	25.04	AAAA
ATOM	1646	CA	GLU	207	17.976	17.373	59.152	1.00	19.61	AAAA
ATOM	1647	CB	GLU	207	18.483	18.322	58.055	1.00	20.75	AAAA
ATOM	1648	CG	GLU	207	17.682	18.222	56.753	1.00	18.44	AAAA
ATOM	1649	CD	GLU	207	17.687	19.514	55.983	1.00	24.75	AAAA
ATOM	1650	OE1	GLU	207	18.738	20.182	55.948	1.00	22.17	AAAA

44/263
Figure 16-26

ATOM	1651	OE2	GLU	207	16.646	19.854	55.396	1.00	15.50	AAAA
ATOM	1652	C	GLU	207	18.921	17.379	60.350	1.00	28.83	AAAA
ATOM	1653	O	GLU	207	19.506	18.416	60.687	1.00	18.11	AAAA
ATOM	1654	N	ILE	208	19.081	16.218	60.988	1.00	21.60	AAAA
ATOM	1655	CA	ILE	208	19.930	16.138	62.168	1.00	22.37	AAAA
ATOM	1656	CB	ILE	208	19.113	15.652	63.403	1.00	28.84	AAAA
ATOM	1657	CG2	ILE	208	19.968	15.693	64.653	1.00	43.26	AAAA
ATOM	1658	CG1	ILE	208	17.905	16.561	63.625	1.00	21.61	AAAA
ATOM	1659	CD1	ILE	208	17.029	16.160	64.786	1.00	41.40	AAAA
ATOM	1660	C	ILE	208	21.156	15.260	61.981	1.00	24.74	AAAA
ATOM	1661	O	ILE	208	21.785	14.850	62.943	1.00	22.68	AAAA
ATOM	1662	N	GLY	209	21.512	14.969	60.738	1.00	22.80	AAAA
ATOM	1663	CA	GLY	209	22.690	14.153	60.535	1.00	20.43	AAAA
ATOM	1664	C	GLY	209	22.342	12.769	60.037	1.00	25.56	AAAA
ATOM	1665	O	GLY	209	21.165	12.447	59.850	1.00	25.22	AAAA
ATOM	1666	N	GLU	210	23.373	11.944	59.888	1.00	26.07	AAAA
ATOM	1667	CA	GLU	210	23.235	10.601	59.348	1.00	25.78	AAAA
ATOM	1668	CB	GLU	210	23.404	10.731	57.835	1.00	28.27	AAAA
ATOM	1669	CG	GLU	210	23.041	9.569	56.965	1.00	56.41	AAAA
ATOM	1670	CD	GLU	210	23.170	9.952	55.495	1.00	65.37	AAAA
ATOM	1671	OE1	GLU	210	24.290	10.327	55.075	1.00	62.00	AAAA
ATOM	1672	OE2	GLU	210	22.153	9.894	54.768	1.00	73.24	AAAA
ATOM	1673	C	GLU	210	24.329	9.709	59.936	1.00	31.85	AAAA
ATOM	1674	O	GLU	210	25.447	10.170	60.217	1.00	28.85	AAAA
ATOM	1675	N	GLY	211	24.012	8.431	60.121	1.00	27.84	AAAA
ATOM	1676	CA	GLY	211	24.991	7.502	60.657	1.00	26.25	AAAA
ATOM	1677	C	GLY	211	25.545	7.942	61.995	1.00	27.79	AAAA
ATOM	1678	O	GLY	211	24.788	8.324	62.874	1.00	28.66	AAAA
ATOM	1679	N	LYS	212	26.865	7.880	62.150	1.00	34.62	AAAA
ATOM	1680	CA	LYS	212	27.512	8.287	63.393	1.00	34.39	AAAA
ATOM	1681	CB	LYS	212	29.029	8.132	63.273	1.00	40.40	AAAA
ATOM	1682	CG	LYS	212	29.505	6.712	62.996	1.00	53.97	AAAA
ATOM	1683	CD	LYS	212	29.139	5.770	64.131	1.00	61.93	AAAA
ATOM	1684	CE	LYS	212	29.612	4.347	63.863	1.00	62.74	AAAA
ATOM	1685	NZ	LYS	212	31.091	4.258	63.711	1.00	70.11	AAAA
ATOM	1686	C	LYS	212	27.181	9.741	63.725	1.00	36.04	AAAA
ATOM	1687	O	LYS	212	27.109	10.126	64.897	1.00	28.34	AAAA
ATOM	1688	N	GLY	213	26.959	10.543	62.688	1.00	31.47	AAAA
ATOM	1689	CA	GLY	213	26.648	11.948	62.898	1.00	31.68	AAAA
ATOM	1690	C	GLY	213	25.189	12.291	63.142	1.00	28.78	AAAA
ATOM	1691	O	GLY	213	24.840	13.460	63.259	1.00	22.56	AAAA
ATOM	1692	N	LYS	214	24.317	11.292	63.222	1.00	28.54	AAAA
ATOM	1693	CA	LYS	214	22.905	11.585	63.463	1.00	31.11	AAAA
ATOM	1694	CB	LYS	214	22.080	10.295	63.325	1.00	31.03	AAAA
ATOM	1695	CG	LYS	214	20.583	10.461	63.224	1.00	38.15	AAAA
ATOM	1696	CD	LYS	214	19.968	9.115	62.844	1.00	40.49	AAAA
ATOM	1697	CE	LYS	214	18.490	9.220	62.537	1.00	48.02	AAAA
ATOM	1698	NZ	LYS	214	17.927	7.924	62.064	1.00	44.99	AAAA
ATOM	1699	C	LYS	214	22.834	12.160	64.875	1.00	26.90	AAAA
ATOM	1700	O	LYS	214	23.260	11.524	65.831	1.00	33.33	AAAA
ATOM	1701	N	GLY	215	22.310	13.376	64.997	1.00	24.38	AAAA
ATOM	1702	CA	GLY	215	22.230	14.034	66.290	1.00	26.03	AAAA
ATOM	1703	C	GLY	215	23.298	15.115	66.447	1.00	27.03	AAAA
ATOM	1704	O	GLY	215	23.352	15.820	67.458	1.00	23.34	AAAA
ATOM	1705	N	TYR	216	24.152	15.260	65.439	1.00	22.79	AAAA
ATOM	1706	CA	TYR	216	25.217	16.257	65.512	1.00	25.51	AAAA
ATOM	1707	CB	TYR	216	26.592	15.576	65.406	1.00	20.54	AAAA
ATOM	1708	CG	TYR	216	26.900	14.671	66.581	1.00	26.47	AAAA
ATOM	1709	CD1	TYR	216	26.221	13.464	66.757	1.00	28.96	AAAA
ATOM	1710	CE1	TYR	216	26.455	12.660	67.872	1.00	33.08	AAAA
ATOM	1711	CD2	TYR	216	27.832	15.052	67.552	1.00	24.21	AAAA
ATOM	1712	CE2	TYR	216	28.074	14.254	68.675	1.00	34.45	AAAA
ATOM	1713	CZ	TYR	216	27.378	13.063	68.827	1.00	40.53	AAAA
ATOM	1714	OH	TYR	216	27.580	12.291	69.947	1.00	45.67	AAAA
ATOM	1715	C	TYR	216	25.104	17.391	64.493	1.00	22.57	AAAA
ATOM	1716	O	TYR	216	26.097	18.014	64.126	1.00	19.70	AAAA

45/263 Figure 16-27

ATOM	1717	N	ASN	217	23.889	17.635	64.027	1.00	22.88	AAAA
ATOM	1718	CA	ASN	217	23.621	18.729	63.109	1.00	22.60	AAAA
ATOM	1719	CB	ASN	217	23.453	18.240	61.671	1.00	16.61	AAAA
ATOM	1720	CG	ASN	217	23.233	19.387	60.695	1.00	17.16	AAAA
ATOM	1721	OD1	ASN	217	22.098	19.704	60.307	1.00	20.23	AAAA
ATOM	1722	ND2	ASN	217	24.320	20.032	60.309	1.00	12.18	AAAA
ATOM	1723	C	ASN	217	22.311	19.296	63.630	1.00	17.65	AAAA
ATOM	1724	O	ASN	217	21.381	18.550	63.894	1.00	17.63	AAAA
ATOM	1725	N	LEU	218	22.236	20.610	63.793	1.00	21.68	AAAA
ATOM	1726	CA	LEU	218	21.014	21.197	64.320	1.00	21.20	AAAA
ATOM	1727	CB	LEU	218	21.186	21.547	65.808	1.00	17.73	AAAA
ATOM	1728	CG	LEU	218	19.906	21.702	66.647	1.00	32.30	AAAA
ATOM	1729	CD1	LEU	218	20.228	22.427	67.944	1.00	24.51	AAAA
ATOM	1730	CD2	LEU	218	18.862	22.464	65.903	1.00	40.08	AAAA
ATOM	1731	C	LEU	218	20.700	22.459	63.554	1.00	19.46	AAAA
ATOM	1732	O	LEU	218	21.467	23.425	63.615	1.00	16.70	AAAA
ATOM	1733	N	ASN	219	19.590	22.441	62.824	1.00	15.43	AAAA
ATOM	1734	CA	ASN	219	19.143	23.609	62.072	1.00	14.05	AAAA
ATOM	1735	CB	ASN	219	18.634	23.232	60.665	1.00	15.92	AAAA
ATOM	1736	CG	ASN	219	19.732	22.738	59.750	1.00	22.73	AAAA
ATOM	1737	OD1	ASN	219	20.861	23.232	59.802	1.00	17.90	AAAA
ATOM	1738	ND2	ASN	219	19.398	21.789	58.868	1.00	16.62	AAAA
ATOM	1739	C	ASN	219	17.990	24.256	62.821	1.00	21.98	AAAA
ATOM	1740	O	ASN	219	17.075	23.569	63.262	1.00	18.65	AAAA
ATOM	1741	N	ILE	220	18.025	25.580	62.952	1.00	16.82	AAAA
ATOM	1742	CA	ILE	220	16.951	26.298	63.640	1.00	13.22	AAAA
ATOM	1743	CB	ILE	220	17.522	27.115	64.823	1.00	15.70	AAAA
ATOM	1744	CG2	ILE	220	16.411	27.912	65.479	1.00	15.18	AAAA
ATOM	1745	CG1	ILE	220	18.246	26.193	65.823	1.00	19.11	AAAA
ATOM	1746	CD1	ILE	220	17.350	25.259	66.632	1.00	22.75	AAAA
ATOM	1747	C	ILE	220	16.363	27.246	62.573	1.00	18.80	AAAA
ATOM	1748	O	ILE	220	16.810	28.386	62.419	1.00	15.52	AAAA
ATOM	1749	N	PRO	221	15.341	26.790	61.826	1.00	16.72	AAAA
ATOM	1750	CD	PRO	221	14.612	25.518	61.906	1.00	18.83	AAAA
ATOM	1751	CA	PRO	221	14.739	27.628	60.785	1.00	19.83	AAAA
ATOM	1752	CB	PRO	221	13.930	26.615	59.948	1.00	20.76	AAAA
ATOM	1753	CG	PRO	221	14.409	25.241	60.462	1.00	28.73	AAAA
ATOM	1754	C	PRO	221	13.849	28.664	61.444	1.00	21.26	AAAA
ATOM	1755	O	PRO	221	13.061	28.318	62.314	1.00	22.46	AAAA
ATOM	1756	N	LEU	222	13.977	29.926	61.028	1.00	19.70	AAAA
ATOM	1757	CA	LEU	222	13.209	31.018	61.612	1.00	21.62	AAAA
ATOM	1758	CB	LEU	222	14.163	31.972	62.319	1.00	16.46	AAAA
ATOM	1759	CG	LEU	222	14.868	31.232	63.466	1.00	18.65	AAAA
ATOM	1760	CD1	LEU	222	16.026	32.072	64.014	1.00	21.32	AAAA
ATOM	1761	CD2	LEU	222	13.857	30.925	64.555	1.00	19.98	AAAA
ATOM	1762	C	LEU	222	12.350	31.763	60.590	1.00	19.68	AAAA
ATOM	1763	O	LEU	222	12.687	31.830	59.412	1.00	18.07	AAAA
ATOM	1764	N	PRO	223	11.220	32.329	61.042	1.00	19.37	AAAA
ATOM	1765	CD	PRO	223	10.723	32.249	62.431	1.00	17.38	AAAA
ATOM	1766	CA	PRO	223	10.264	33.065	60.203	1.00	19.59	AAAA
ATOM	1767	CB	PRO	223	9.006	33.083	61.074	1.00	20.08	AAAA
ATOM	1768	CG	PRO	223	9.608	33.304	62.441	1.00	21.96	AAAA
ATOM	1769	C	PRO	223	10.606	34.458	59.723	1.00	23.15	AAAA
ATOM	1770	O	PRO	223	11.525	35.101	60.214	1.00	15.81	AAAA
ATOM	1771	N	LYS	224	9.830	34.912	58.745	1.00	16.41	AAAA
ATOM	1772	CA	LYS	224	9.975	36.254	58.200	1.00	16.11	AAAA
ATOM	1773	CB	LYS	224	9.002	36.446	57.039	1.00	20.34	AAAA
ATOM	1774	CG	LYS	224	9.163	35.441	55.900	1.00	19.33	AAAA
ATOM	1775	CD	LYS	224	8.109	35.687	54.807	1.00	25.49	AAAA
ATOM	1776	CE	LYS	224	8.209	34.624	53.704	1.00	24.14	AAAA
ATOM	1777	NZ	LYS	224	7.207	34.843	52.618	1.00	34.08	AAAA
ATOM	1778	C	LYS	224	9.638	37.289	59.284	1.00	15.77	AAAA
ATOM	1779	O	LYS	224	8.819	37.032	60.186	1.00	21.07	AAAA
ATOM	1780	N	GLY	225	10.239	38.469	59.171	1.00	20.77	AAAA
ATOM	1781	CA	GLY	225	9.974	39.527	60.129	1.00	20.30	AAAA
ATOM	1782	C	GLY	225	10.556	39.286	61.507	1.00	20.63	AAAA

46/263

Figure 16-28

ATOM	1783	O	GLY	225	10.128	39.912	62.468	1.00	20.66	AAAA
ATOM	1784	N	LEU	226	11.540	38.395	61.606	1.00	20.37	AAAA
ATOM	1785	CA	LEU	226	12.154	38.063	62.893	1.00	18.71	AAAA
ATOM	1786	CB	LEU	226	13.354	37.145	62.670	1.00	13.63	AAAA
ATOM	1787	CG	LEU	226	13.836	36.443	63.939	1.00	18.44	AAAA
ATOM	1788	CD1	LEU	226	12.834	35.329	64.243	1.00	18.09	AAAA
ATOM	1789	CD2	LEU	226	15.232	35.844	63.741	1.00	17.96	AAAA
ATOM	1790	C	LEU	226	12.649	39.309	63.642	1.00	19.84	AAAA
ATOM	1791	O	LEU	226	13.320	40.151	63.052	1.00	18.13	AAAA
ATOM	1792	N	ASN	227	12.336	39.421	64.932	1.00	23.30	AAAA
ATOM	1793	CA	ASN	227	12.815	40.571	65.692	1.00	20.88	AAAA
ATOM	1794	CB	ASN	227	11.682	41.261	66.485	1.00	21.73	AAAA
ATOM	1795	CG	ASN	227	11.061	40.368	67.546	1.00	20.47	AAAA
ATOM	1796	OD1	ASN	227	11.762	39.736	68.341	1.00	23.80	AAAA
ATOM	1797	ND2	ASN	227	9.729	40.340	67.581	1.00	21.08	AAAA
ATOM	1798	C	ASN	227	13.950	40.152	66.612	1.00	25.24	AAAA
ATOM	1799	O	ASN	227	14.282	38.965	66.702	1.00	18.54	AAAA
ATOM	1800	N	ASP	228	14.547	41.124	67.296	1.00	19.41	AAAA
ATOM	1801	CA	ASP	228	15.682	40.844	68.169	1.00	22.15	AAAA
ATOM	1802	CB	ASP	228	16.208	42.141	68.802	1.00	16.82	AAAA
ATOM	1803	CG	ASP	228	16.852	43.060	67.796	1.00	30.68	AAAA
ATOM	1804	OD1	ASP	228	17.182	42.576	66.690	1.00	23.87	AAAA
ATOM	1805	OD2	ASP	228	17.053	44.256	68.123	1.00	25.02	AAAA
ATOM	1806	C	ASP	228	15.440	39.835	69.265	1.00	18.83	AAAA
ATOM	1807	O	ASP	228	16.298	39.002	69.536	1.00	16.28	AAAA
ATOM	1808	N	ASN	229	14.291	39.930	69.928	1.00	20.73	AAAA
ATOM	1809	CA	ASN	229	13.975	39.015	71.007	1.00	21.75	AAAA
ATOM	1810	CB	ASN	229	12.706	39.483	71.712	1.00	19.46	AAAA
ATOM	1811	CG	ASN	229	12.943	40.738	72.516	1.00	27.14	AAAA
ATOM	1812	OD1	ASN	229	13.588	40.691	73.556	1.00	33.03	AAAA
ATOM	1813	ND2	ASN	229	12.464	41.874	72.019	1.00	21.35	AAAA
ATOM	1814	C	ASN	229	13.833	37.596	70.503	1.00	18.47	AAAA
ATOM	1815	O	ASN	229	14.284	36.644	71.151	1.00	22.47	AAAA
ATOM	1816	N	GLU	230	13.252	37.454	69.319	1.00	17.79	AAAA
ATOM	1817	CA	GLU	230	13.081	36.125	68.748	1.00	21.18	AAAA
ATOM	1818	CB	GLU	230	12.152	36.193	67.536	1.00	20.54	AAAA
ATOM	1819	CG	GLU	230	10.765	36.714	67.890	1.00	28.98	AAAA
ATOM	1820	CD	GLU	230	9.870	36.816	66.677	1.00	24.35	AAAA
ATOM	1821	OE1	GLU	230	10.360	37.296	65.638	1.00	22.00	AAAA
ATOM	1822	OE2	GLU	230	8.683	36.443	66.772	1.00	24.99	AAAA
ATOM	1823	C	GLU	230	14.422	35.507	68.361	1.00	16.89	AAAA
ATOM	1824	O	GLU	230	14.663	34.326	68.603	1.00	19.45	AAAA
ATOM	1825	N	PHE	231	15.305	36.305	67.772	1.00	15.68	AAAA
ATOM	1826	CA	PHE	231	16.616	35.788	67.389	1.00	15.78	AAAA
ATOM	1827	CB	PHE	231	17.420	36.863	66.649	1.00	13.22	AAAA
ATOM	1828	CG	PHE	231	18.719	36.361	66.069	1.00	20.63	AAAA
ATOM	1829	CD1	PHE	231	18.723	35.445	65.016	1.00	18.42	AAAA
ATOM	1830	CD2	PHE	231	19.936	36.804	66.568	1.00	21.10	AAAA
ATOM	1831	CE1	PHE	231	19.918	34.983	64.471	1.00	17.67	AAAA
ATOM	1832	CE2	PHE	231	21.144	36.346	66.029	1.00	28.29	AAAA
ATOM	1833	CZ	PHE	231	21.130	35.431	64.976	1.00	27.85	AAAA
ATOM	1834	C	PHE	231	17.385	35.332	68.636	1.00	18.54	AAAA
ATOM	1835	O	PHE	231	17.869	34.201	68.702	1.00	18.86	AAAA
ATOM	1836	N	LEU	232	17.495	36.204	69.636	1.00	19.07	AAAA
ATOM	1837	CA	LEU	232	18.239	35.850	70.848	1.00	17.39	AAAA
ATOM	1838	CB	LEU	232	18.415	37.078	71.737	1.00	24.53	AAAA
ATOM	1839	CG	LEU	232	19.214	38.202	71.061	1.00	16.64	AAAA
ATOM	1840	CD1	LEU	232	19.134	39.449	71.934	1.00	26.70	AAAA
ATOM	1841	CD2	LEU	232	20.659	37.806	70.810	1.00	18.77	AAAA
ATOM	1842	C	LEU	232	17.607	34.707	71.628	1.00	19.82	AAAA
ATOM	1843	O	LEU	232	18.309	33.904	72.217	1.00	21.80	AAAA
ATOM	1844	N	PHE	233	16.281	34.640	71.648	1.00	17.18	AAAA
ATOM	1845	CA	PHE	233	15.587	33.537	72.309	1.00	23.34	AAAA
ATOM	1846	CB	PHE	233	14.074	33.663	72.095	1.00	19.17	AAAA
ATOM	1847	CG	PHE	233	13.289	32.447	72.523	1.00	21.40	AAAA
ATOM	1848	CD1	PHE	233	12.863	32.302	73.841	1.00	29.62	AAAA

47/263 Figure 16-29

ATOM	1849	CD2	PHE	233	12.942	31.473	71.596	1.00	19.92	AAAA
ATOM	1850	CE1	PHE	233	12.088	31.206	74.229	1.00	29.35	AAAA
ATOM	1851	CE2	PHE	233	12.168	30.363	71.966	1.00	25.37	AAAA
ATOM	1852	CZ	PHE	233	11.737	30.231	73.283	1.00	30.28	AAAA
ATOM	1853	C	PHE	233	16.041	32.234	71.660	1.00	23.12	AAAA
ATOM	1854	O	PHE	233	16.433	31.273	72.332	1.00	18.35	AAAA
ATOM	1855	N	ALA	234	15.961	32.208	70.332	1.00	17.26	AAAA
ATOM	1856	CA	ALA	234	16.332	31.026	69.562	1.00	17.67	AAAA
ATOM	1857	CB	ALA	234	16.085	31.297	68.046	1.00	19.08	AAAA
ATOM	1858	C	ALA	234	17.786	30.641	69.800	1.00	16.31	AAAA
ATOM	1859	O	ALA	234	18.127	29.461	69.926	1.00	16.75	AAAA
ATOM	1860	N	LEU	235	18.646	31.643	69.846	1.00	16.73	AAAA
ATOM	1861	CA	LEU	235	20.074	31.411	70.051	1.00	19.14	AAAA
ATOM	1862	CB	LEU	235	20.823	32.742	69.956	1.00	21.72	AAAA
ATOM	1863	CG	LEU	235	22.226	32.790	69.345	1.00	36.73	AAAA
ATOM	1864	CD1	LEU	235	23.026	33.844	70.105	1.00	20.69	AAAA
ATOM	1865	CD2	LEU	235	22.917	31.426	69.393	1.00	22.96	AAAA
ATOM	1866	C	LEU	235	20.354	30.776	71.421	1.00	18.71	AAAA
ATOM	1867	O	LEU	235	21.028	29.747	71.522	1.00	18.59	AAAA
ATOM	1868	N	GLU	236	19.831	31.390	72.479	1.00	25.43	AAAA
ATOM	1869	CA	GLU	236	20.046	30.883	73.839	1.00	19.75	AAAA
ATOM	1870	CB	GLU	236	19.335	31.777	74.860	1.00	23.18	AAAA
ATOM	1871	CG	GLU	236	19.725	33.229	74.777	1.00	38.53	AAAA
ATOM	1872	CD	GLU	236	18.857	34.119	75.648	1.00	42.42	AAAA
ATOM	1873	OE1	GLU	236	17.617	34.171	75.428	1.00	45.43	AAAA
ATOM	1874	OE2	GLU	236	19.425	34.768	76.548	1.00	48.76	AAAA
ATOM	1875	C	GLU	236	19.541	29.452	74.011	1.00	25.85	AAAA
ATOM	1876	O	GLU	236	20.222	28.603	74.597	1.00	21.36	AAAA
ATOM	1877	N	LYS	237	20.222	28.603	74.597	1.00	21.36	AAAA
ATOM	1878	CA	LYS	237	18.343	29.193	73.501	1.00	23.16	AAAA
ATOM	1879	CB	LYS	237	17.752	27.871	73.610	1.00	17.06	AAAA
ATOM	1880	CG	LYS	237	16.282	27.943	73.193	1.00	26.98	AAAA
ATOM	1881	CD	LYS	237	15.483	26.711	73.519	1.00	52.00	AAAA
ATOM	1882	CE	LYS	237	14.078	27.110	73.932	1.00	56.40	AAAA
ATOM	1883	NZ	LYS	237	14.131	27.979	75.183	1.00	52.03	AAAA
ATOM	1884	C	LYS	237	12.782	28.421	75.614	1.00	55.53	AAAA
ATOM	1885	O	LYS	237	18.502	26.827	72.785	1.00	18.46	AAAA
ATOM	1886	N	SER	238	18.691	25.692	73.231	1.00	21.20	AAAA
ATOM	1887	CA	SER	238	18.932	27.187	71.578	1.00	21.28	AAAA
ATOM	1888	CB	SER	238	19.649	26.208	70.776	1.00	16.47	AAAA
ATOM	1889	OG	SER	238	19.745	26.666	69.307	1.00	19.75	AAAA
ATOM	1890	C	SER	238	20.475	27.858	69.160	1.00	22.52	AAAA
ATOM	1891	O	SER	238	21.039	25.923	71.361	1.00	18.79	AAAA
ATOM	1892	N	LEU	239	21.521	24.788	71.312	1.00	20.60	AAAA
ATOM	1893	CA	LEU	239	21.690	26.937	71.925	1.00	22.95	AAAA
ATOM	1894	CB	LEU	239	23.004	26.701	72.513	1.00	20.98	AAAA
ATOM	1895	CG	LEU	239	23.652	28.008	72.986	1.00	18.39	AAAA
ATOM	1896	CD1	LEU	239	23.985	29.072	71.933	1.00	20.02	AAAA
ATOM	1897	CD2	LEU	239	24.538	30.311	72.636	1.00	27.02	AAAA
ATOM	1898	C	LEU	239	25.010	28.556	70.933	1.00	20.31	AAAA
ATOM	1899	O	LEU	239	22.882	25.735	73.680	1.00	25.16	AAAA
ATOM	1900	N	GLU	240	23.780	24.929	73.920	1.00	20.70	AAAA
ATOM	1901	CA	GLU	240	21.768	25.800	74.398	1.00	24.93	AAAA
ATOM	1902	CB	GLU	240	21.570	24.912	75.536	1.00	25.72	AAAA
ATOM	1903	CG	GLU	240	20.331	25.356	76.337	1.00	29.10	AAAA
ATOM	1904	CD	GLU	240	20.042	24.531	77.581	1.00	49.56	AAAA
ATOM	1905	OE1	GLU	240	19.053	25.212	78.515	1.00	63.15	AAAA
ATOM	1906	OE2	GLU	240	17.935	25.550	78.067	1.00	69.26	AAAA
ATOM	1907	C	GLU	240	19.400	25.410	79.703	1.00	66.68	AAAA
ATOM	1908	O	GLU	240	21.440	23.469	75.046	1.00	23.44	AAAA
ATOM	1909	N	ILE	241	21.951	22.535	75.674	1.00	23.10	AAAA
ATOM	1910	CA	ILE	241	20.771	23.294	73.913	1.00	19.52	AAAA
ATOM	1911	CB	ILE	241	20.598	21.978	73.321	1.00	24.06	AAAA
ATOM	1912	CG2	ILE	241	19.705	22.039	72.052	1.00	23.80	AAAA
ATOM	1913	CG1	ILE	241	19.718	20.678	71.323	1.00	24.94	AAAA
ATOM	1914	CD1	ILE	241	18.281	22.433	72.439	1.00	28.60	AAAA
ATOM					17.336	22.600	71.257	1.00	27.04	AAAA

ATOM	1915	C	ILE	241	21.957	21.404	72.941	1.00	25.48	AAAA
ATOM	1916	O	ILE	241	22.244	20.234	73.195	1.00	19.43	AAAA
ATOM	1917	N	VAL	242	22.799	22.235	72.334	1.00	20.41	AAAA
ATOM	1918	CA	VAL	242	24.116	21.782	71.928	1.00	23.17	AAAA
ATOM	1919	CB	VAL	242	24.853	22.856	71.107	1.00	26.48	AAAA
ATOM	1920	CG1	VAL	242	26.273	22.394	70.807	1.00	18.67	AAAA
ATOM	1921	CG2	VAL	242	24.093	23.135	69.802	1.00	26.97	AAAA
ATOM	1922	C	VAL	242	24.962	21.456	73.154	1.00	24.81	AAAA
ATOM	1923	O	VAL	242	25.566	20.384	73.235	1.00	22.49	AAAA
ATOM	1924	N	LYS	243	24.989	22.387	74.102	1.00	26.06	AAAA
ATOM	1925	CA	LYS	243	25.775	22.202	75.311	1.00	32.57	AAAA
ATOM	1926	CB	LYS	243	25.599	23.379	76.272	1.00	28.53	AAAA
ATOM	1927	CG	LYS	243	26.386	23.183	77.568	1.00	43.21	AAAA
ATOM	1928	CD	LYS	243	26.022	24.191	78.653	1.00	53.10	AAAA
ATOM	1929	CE	LYS	243	26.407	25.607	78.287	1.00	50.30	AAAA
ATOM	1930	NZ	LYS	243	26.045	26.548	79.389	1.00	59.15	AAAA
ATOM	1931	C	LYS	243	25.433	20.917	76.046	1.00	30.38	AAAA
ATOM	1932	O	LYS	243	26.321	20.255	76.578	1.00	35.44	AAAA
ATOM	1933	N	GLU	244	24.161	20.542	76.076	1.00	28.12	AAAA
ATOM	1934	CA	GLU	244	23.798	19.320	76.798	1.00	37.54	AAAA
ATOM	1935	CB	GLU	244	22.288	19.260	77.048	1.00	35.34	AAAA
ATOM	1936	CG	GLU	244	21.735	20.459	77.816	1.00	55.88	AAAA
ATOM	1937	CD	GLU	244	20.281	20.275	78.230	1.00	57.89	AAAA
ATOM	1938	OE1	GLU	244	19.673	21.246	78.738	1.00	60.60	AAAA
ATOM	1939	OE2	GLU	244	19.753	19.152	78.062	1.00	57.73	AAAA
ATOM	1940	C	GLU	244	24.231	18.034	76.102	1.00	38.17	AAAA
ATOM	1941	O	GLU	244	24.294	16.978	76.727	1.00	38.46	AAAA
ATOM	1942	N	VAL	245	24.541	18.124	74.817	1.00	30.29	AAAA
ATOM	1943	CA	VAL	245	24.933	16.958	74.042	1.00	39.17	AAAA
ATOM	1944	CB	VAL	245	23.984	16.778	72.833	1.00	46.68	AAAA
ATOM	1945	CG1	VAL	245	24.462	15.641	71.942	1.00	53.09	AAAA
ATOM	1946	CG2	VAL	245	22.581	16.488	73.327	1.00	54.19	AAAA
ATOM	1947	C	VAL	245	26.364	16.982	73.508	1.00	34.90	AAAA
ATOM	1948	O	VAL	245	26.915	15.939	73.164	1.00	34.73	AAAA
ATOM	1949	N	PHE	246	26.980	18.156	73.465	1.00	29.22	AAAA
ATOM	1950	CA	PHE	246	28.324	18.256	72.897	1.00	29.17	AAAA
ATOM	1951	CB	PHE	246	28.178	18.800	71.464	1.00	30.42	AAAA
ATOM	1952	CG	PHE	246	29.384	18.588	70.585	1.00	25.62	AAAA
ATOM	1953	CD1	PHE	246	29.695	17.326	70.097	1.00	28.89	AAAA
ATOM	1954	CD2	PHE	246	30.167	19.668	70.196	1.00	25.17	AAAA
ATOM	1955	CE1	PHE	246	30.771	17.138	69.222	1.00	23.43	AAAA
ATOM	1956	CE2	PHE	246	31.248	19.495	69.322	1.00	22.40	AAAA
ATOM	1957	CZ	PHE	246	31.549	18.236	68.835	1.00	19.88	AAAA
ATOM	1958	C	PHE	246	29.233	19.176	73.712	1.00	23.38	AAAA
ATOM	1959	O	PHE	246	28.867	20.312	74.002	1.00	29.15	AAAA
ATOM	1960	N	GLU	247	30.410	18.682	74.094	1.00	29.73	AAAA
ATOM	1961	CA	GLU	247	31.395	19.481	74.841	1.00	28.10	AAAA
ATOM	1962	CB	GLU	247	31.912	18.726	76.074	1.00	35.75	AAAA
ATOM	1963	CG	GLU	247	30.972	18.707	77.286	1.00	60.78	AAAA
ATOM	1964	CD	GLU	247	29.700	17.892	77.077	1.00	70.07	AAAA
ATOM	1965	OE1	GLU	247	28.913	18.220	76.165	1.00	79.95	AAAA
ATOM	1966	OE2	GLU	247	29.481	16.920	77.835	1.00	76.80	AAAA
ATOM	1967	C	GLU	247	32.554	19.741	73.876	1.00	28.90	AAAA
ATOM	1968	O	GLU	247	33.490	18.946	73.778	1.00	23.67	AAAA
ATOM	1969	N	PRO	248	32.531	20.891	73.181	1.00	25.02	AAAA
ATOM	1970	CD	PRO	248	31.574	22.003	73.310	1.00	27.23	AAAA
ATOM	1971	CA	PRO	248	33.566	21.249	72.209	1.00	28.06	AAAA
ATOM	1972	CB	PRO	248	33.050	22.575	71.639	1.00	28.11	AAAA
ATOM	1973	CG	PRO	248	31.551	22.512	71.897	1.00	34.57	AAAA
ATOM	1974	C	PRO	248	34.968	21.416	72.770	1.00	23.87	AAAA
ATOM	1975	O	PRO	248	35.132	21.897	73.887	1.00	24.05	AAAA
ATOM	1976	N	GLU	249	35.965	21.013	71.983	1.00	24.34	AAAA
ATOM	1977	CA	GLU	249	37.366	21.195	72.355	1.00	25.98	AAAA
ATOM	1978	CB	GLU	249	38.275	20.166	71.679	1.00	22.07	AAAA
ATOM	1979	CG	GLU	249	38.046	18.726	72.116	1.00	33.40	AAAA
ATOM	1980	CD	GLU	249	39.005	17.767	71.445	1.00	29.15	AAAA

Figure 16-31

ATOM	1981	OE1	GLU	249	39.071	17.770	70.199	1.00	27.62	AAAA
ATOM	1982	OE2	GLU	249	39.694	17.004	72.161	1.00	26.19	AAAA
ATOM	1983	C	GLU	249	37.692	22.561	71.786	1.00	26.04	AAAA
ATOM	1984	O	GLU	249	38.582	23.271	72.262	1.00	26.39	AAAA
ATOM	1985	N	VAL	250	36.953	22.921	70.744	1.00	23.83	AAAA
ATOM	1986	CA	VAL	250	37.151	24.197	70.086	1.00	19.67	AAAA
ATOM	1987	CB	VAL	250	38.438	24.178	69.210	1.00	20.88	AAAA
ATOM	1988	CG1	VAL	250	38.348	23.117	68.128	1.00	18.18	AAAA
ATOM	1989	CG2	VAL	250	38.647	25.530	68.591	1.00	16.71	AAAA
ATOM	1990	C	VAL	250	35.946	24.483	69.207	1.00	20.78	AAAA
ATOM	1991	O	VAL	250	35.299	23.556	68.746	1.00	19.60	AAAA
ATOM	1992	N	TYR	251	35.633	25.757	69.000	1.00	18.75	AAAA
ATOM	1993	CA	TYR	251	34.497	26.109	68.153	1.00	22.44	AAAA
ATOM	1994	CB	TYR	251	33.261	26.437	69.022	1.00	16.57	AAAA
ATOM	1995	CG	TYR	251	33.207	27.856	69.575	1.00	22.36	AAAA
ATOM	1996	CD1	TYR	251	32.654	28.896	68.823	1.00	18.12	AAAA
ATOM	1997	CE1	TYR	251	32.612	30.185	69.308	1.00	20.40	AAAA
ATOM	1998	CD2	TYR	251	33.715	28.160	70.842	1.00	20.04	AAAA
ATOM	1999	CE2	TYR	251	33.676	29.475	71.349	1.00	16.60	AAAA
ATOM	2000	CZ	TYR	251	33.128	30.473	70.573	1.00	14.68	AAAA
ATOM	2001	OH	TYR	251	33.100	31.780	71.011	1.00	21.79	AAAA
ATOM	2002	C	TYR	251	34.811	27.294	67.236	1.00	20.28	AAAA
ATOM	2003	O	TYR	251	35.695	28.107	67.525	1.00	19.91	AAAA
ATOM	2004	N	LEU	252	34.097	27.360	66.109	1.00	17.90	AAAA
ATOM	2005	CA	LEU	252	34.216	28.466	65.161	1.00	18.58	AAAA
ATOM	2006	CB	LEU	252	34.679	28.001	63.767	1.00	17.55	AAAA
ATOM	2007	CG	LEU	252	36.028	27.290	63.718	1.00	23.36	AAAA
ATOM	2008	CD1	LEU	252	35.819	25.820	64.017	1.00	27.78	AAAA
ATOM	2009	CD2	LEU	252	36.631	27.440	62.331	1.00	27.29	AAAA
ATOM	2010	C	LEU	252	32.816	29.049	65.052	1.00	15.49	AAAA
ATOM	2011	O	LEU	252	31.819	28.320	65.120	1.00	18.82	AAAA
ATOM	2012	N	LEU	253	32.756	30.360	64.891	1.00	16.80	AAAA
ATOM	2013	CA	LEU	253	31.498	31.105	64.817	1.00	17.50	AAAA
ATOM	2014	CB	LEU	253	31.379	31.987	66.073	1.00	15.49	AAAA
ATOM	2015	CG	LEU	253	30.326	33.085	66.165	1.00	17.75	AAAA
ATOM	2016	CD1	LEU	253	28.946	32.438	66.172	1.00	20.85	AAAA
ATOM	2017	CD2	LEU	253	30.536	33.897	67.464	1.00	19.05	AAAA
ATOM	2018	C	LEU	253	31.516	31.985	63.580	1.00	20.22	AAAA
ATOM	2019	O	LEU	253	32.474	32.727	63.371	1.00	18.14	AAAA
ATOM	2020	N	GLN	254	30.466	31.913	62.765	1.00	16.50	AAAA
ATOM	2021	CA	GLN	254	30.411	32.730	61.556	1.00	16.48	AAAA
ATOM	2022	CB	GLN	254	30.085	31.863	60.312	1.00	25.58	AAAA
ATOM	2023	CG	GLN	254	28.647	31.798	59.871	1.00	36.40	AAAA
ATOM	2024	CD	GLN	254	28.337	32.728	58.701	1.00	33.18	AAAA
ATOM	2025	OE1	GLN	254	28.744	32.487	57.546	1.00	21.05	AAAA
ATOM	2026	NE2	GLN	254	27.613	33.799	58.992	1.00	22.85	AAAA
ATOM	2027	C	GLN	254	29.384	33.816	61.832	1.00	16.12	AAAA
ATOM	2028	O	GLN	254	28.282	33.577	62.364	1.00	13.97	AAAA
ATOM	2029	N	LEU	255	29.768	35.032	61.468	1.00	14.42	AAAA
ATOM	2030	CA	LEU	255	28.988	36.215	61.763	1.00	17.99	AAAA
ATOM	2031	CB	LEU	255	29.834	37.070	62.719	1.00	20.68	AAAA
ATOM	2032	CG	LEU	255	30.240	36.283	63.964	1.00	22.90	AAAA
ATOM	2033	CD1	LEU	255	31.446	36.906	64.635	1.00	29.36	AAAA
ATOM	2034	CD2	LEU	255	29.042	36.214	64.900	1.00	14.80	AAAA
ATOM	2035	C	LEU	255	28.541	37.060	60.594	1.00	19.32	AAAA
ATOM	2036	O	LEU	255	28.838	38.260	60.561	1.00	21.23	AAAA
ATOM	2037	N	GLY	256	27.827	36.467	59.639	1.00	17.21	AAAA
ATOM	2038	CA	GLY	256	27.347	37.259	58.516	1.00	15.64	AAAA
ATOM	2039	C	GLY	256	26.413	38.348	59.028	1.00	17.31	AAAA
ATOM	2040	O	GLY	256	25.717	38.150	60.027	1.00	15.62	AAAA
ATOM	2041	N	THR	257	26.389	39.494	58.348	1.00	19.72	AAAA
ATOM	2042	CA	THR	257	25.536	40.598	58.776	1.00	19.88	AAAA
ATOM	2043	CB	THR	257	26.242	41.973	58.589	1.00	14.02	AAAA
ATOM	2044	CG1	THR	257	26.538	42.187	57.206	1.00	17.58	AAAA
ATOM	2045	CG2	THR	257	27.543	42.009	59.392	1.00	19.67	AAAA
ATOM	2046	C	THR	257	24.199	40.634	58.053	1.00	20.58	AAAA

50/263

Figure 16-32

ATOM	2047	O	THR	257	23.403	41.545	58.266	1.00	14.59	AAAA
ATOM	2048	N	ASP	258	23.927	39.639	57.213	1.00	16.56	AAAA
ATOM	2049	CA	ASP	258	22.651	39.646	56.525	1.00	16.39	AAAA
ATOM	2050	CB	ASP	258	22.604	38.611	55.388	1.00	18.38	AAAA
ATOM	2051	CG	ASP	258	23.037	37.229	55.811	1.00	25.85	AAAA
ATOM	2052	OD1	ASP	258	23.222	36.995	57.022	1.00	22.32	AAAA
ATOM	2053	OD2	ASP	258	23.187	36.370	54.909	1.00	18.12	AAAA
ATOM	2054	C	ASP	258	21.396	39.563	57.397	1.00	21.25	AAAA
ATOM	2055	O	ASP	258	20.300	39.781	56.897	1.00	22.52	AAAA
ATOM	2056	N	PRO	259	21.510	39.172	58.680	1.00	18.17	AAAA
ATOM	2057	CD	PRO	259	22.614	38.528	59.422	1.00	25.88	AAAA
ATOM	2058	CA	PRO	259	20.281	39.139	59.482	1.00	21.24	AAAA
ATOM	2059	CB	PRO	259	20.710	38.363	60.735	1.00	21.18	AAAA
ATOM	2060	CG	PRO	259	22.174	38.707	60.846	1.00	36.11	AAAA
ATOM	2061	C	PRO	259	19.705	40.534	59.820	1.00	20.88	AAAA
ATOM	2062	O	PRO	259	18.572	40.647	60.280	1.00	19.25	AAAA
ATOM	2063	N	LEU	260	20.473	41.591	59.571	1.00	18.75	AAAA
ATOM	2064	CA	LEU	260	20.023	42.949	59.875	1.00	22.16	AAAA
ATOM	2065	CB	LEU	260	21.202	43.935	59.778	1.00	20.35	AAAA
ATOM	2066	CG	LEU	260	22.403	43.640	60.682	1.00	21.82	AAAA
ATOM	2067	CD1	LEU	260	23.604	44.486	60.253	1.00	18.57	AAAA
ATOM	2068	CD2	LEU	260	22.032	43.873	62.123	1.00	19.18	AAAA
ATOM	2069	C	LEU	260	18.876	43.469	59.014	1.00	24.16	AAAA
ATOM	2070	O	LEU	260	18.742	43.144	57.826	1.00	21.69	AAAA
ATOM	2071	N	LEU	261	18.049	44.300	59.634	1.00	19.54	AAAA
ATOM	2072	CA	LEU	261	16.903	44.913	58.965	1.00	17.34	AAAA
ATOM	2073	CB	LEU	261	16.285	45.967	59.892	1.00	19.96	AAAA
ATOM	2074	CG	LEU	261	15.204	46.879	59.300	1.00	29.99	AAAA
ATOM	2075	CD1	LEU	261	14.080	46.040	58.732	1.00	33.66	AAAA
ATOM	2076	CD2	LEU	261	14.682	47.819	60.376	1.00	44.71	AAAA
ATOM	2077	C	LEU	261	17.262	45.550	57.620	1.00	18.11	AAAA
ATOM	2078	O	LEU	261	16.539	45.386	56.634	1.00	19.02	AAAA
ATOM	2079	N	GLU	262	18.391	46.249	57.566	1.00	22.68	AAAA
ATOM	2080	CA	GLU	262	18.802	46.921	56.338	1.00	18.46	AAAA
ATOM	2081	CB	GLU	262	19.875	47.965	56.641	1.00	22.01	AAAA
ATOM	2082	CG	GLU	262	19.365	49.136	57.443	1.00	22.94	AAAA
ATOM	2083	CD	GLU	262	19.434	48.902	58.927	1.00	23.11	AAAA
ATOM	2084	OE1	GLU	262	19.668	47.748	59.357	1.00	24.58	AAAA
ATOM	2085	OE2	GLU	262	19.238	49.883	59.667	1.00	27.06	AAAA
ATOM	2086	C	GLU	262	19.281	46.034	55.197	1.00	25.65	AAAA
ATOM	2087	O	GLU	262	19.446	46.510	54.070	1.00	25.49	AAAA
ATOM	2088	N	ASP	263	19.501	44.750	55.467	1.00	22.45	AAAA
ATOM	2089	CA	ASP	263	19.959	43.851	54.418	1.00	15.93	AAAA
ATOM	2090	CB	ASP	263	20.981	42.859	54.988	1.00	18.99	AAAA
ATOM	2091	CG	ASP	263	21.706	42.081	53.907	1.00	22.21	AAAA
ATOM	2092	OD1	ASP	263	22.876	41.730	54.139	1.00	23.19	AAAA
ATOM	2093	OD2	ASP	263	21.112	41.809	52.838	1.00	25.02	AAAA
ATOM	2094	C	ASP	263	18.733	43.165	53.837	1.00	22.32	AAAA
ATOM	2095	O	ASP	263	18.012	42.419	54.519	1.00	18.50	AAAA
ATOM	2096	N	TYR	264	18.500	43.447	52.564	1.00	25.21	AAAA
ATOM	2097	CA	TYR	264	17.339	42.936	51.865	1.00	29.92	AAAA
ATOM	2098	CB	TYR	264	17.077	43.776	50.596	1.00	38.48	AAAA
ATOM	2099	CG	TYR	264	17.910	43.431	49.379	1.00	54.09	AAAA
ATOM	2100	CD1	TYR	264	17.677	42.249	48.660	1.00	69.38	AAAA
ATOM	2101	CE1	TYR	264	18.420	41.930	47.526	1.00	68.71	AAAA
ATOM	2102	CD2	TYR	264	18.915	44.286	48.928	1.00	66.09	AAAA
ATOM	2103	CE2	TYR	264	19.670	43.975	47.788	1.00	74.50	AAAA
ATOM	2104	CZ	TYR	264	19.415	42.794	47.094	1.00	72.57	AAAA
ATOM	2105	OH	TYR	264	20.154	42.472	45.975	1.00	71.96	AAAA
ATOM	2106	C	TYR	264	17.445	41.461	51.532	1.00	29.55	AAAA
ATOM	2107	O	TYR	264	16.448	40.839	51.190	1.00	30.11	AAAA
ATOM	2108	N	LEU	265	18.639	40.891	51.629	1.00	24.45	AAAA
ATOM	2109	CA	LEU	265	18.753	39.476	51.337	1.00	25.36	AAAA
ATOM	2110	CB	LEU	265	20.186	39.089	50.969	1.00	29.81	AAAA
ATOM	2111	CG	LEU	265	20.509	39.510	49.531	1.00	34.43	AAAA
ATOM	2112	CD1	LEU	265	21.847	38.930	49.100	1.00	44.38	AAAA

51/263
Figure 16-33

ATOM	2113	CD2	LEU	265	19.422	38.990	48.603	1.00	46.72	AAAA
ATOM	2114	C	LEU	265	18.209	38.585	52.447	1.00	22.33	AAAA
ATOM	2115	O	LEU	265	18.279	37.364	52.348	1.00	23.48	AAAA
ATOM	2116	N	SER	266	17.677	39.194	53.508	1.00	17.50	AAAA
ATOM	2117	CA	SER	266	17.055	38.398	54.569	1.00	19.69	AAAA
ATOM	2118	CB	SER	266	17.912	38.314	55.845	1.00	20.73	AAAA
ATOM	2119	OG	SER	266	17.696	39.442	56.684	1.00	22.81	AAAA
ATOM	2120	C	SER	266	15.739	39.048	54.950	1.00	19.75	AAAA
ATOM	2121	O	SER	266	15.572	40.265	54.840	1.00	23.66	AAAA
ATOM	2122	N	LYS	267	14.799	38.229	55.402	1.00	18.40	AAAA
ATOM	2123	CA	LYS	267	13.527	38.759	55.851	1.00	20.64	AAAA
ATOM	2124	CB	LYS	267	12.397	37.787	55.513	1.00	20.96	AAAA
ATOM	2125	CG	LYS	267	12.269	37.536	54.025	1.00	25.60	AAAA
ATOM	2126	CD	LYS	267	12.095	38.823	53.259	1.00	33.47	AAAA
ATOM	2127	CE	LYS	267	11.985	38.540	51.772	1.00	38.49	AAAA
ATOM	2128	NZ	LYS	267	11.954	39.793	50.991	1.00	33.11	AAAA
ATOM	2129	C	LYS	267	13.601	38.987	57.365	1.00	20.63	AAAA
ATOM	2130	O	LYS	267	12.584	39.192	58.017	1.00	25.38	AAAA
ATOM	2131	N	PHE	268	14.814	38.937	57.915	1.00	18.98	AAAA
ATOM	2132	CA	PHE	268	15.034	39.182	59.345	1.00	18.50	AAAA
ATOM	2133	CB	PHE	268	16.328	38.510	59.833	1.00	20.91	AAAA
ATOM	2134	CG	PHE	268	16.252	37.006	59.967	1.00	16.96	AAAA
ATOM	2135	CD1	PHE	268	17.374	36.290	60.415	1.00	16.61	AAAA
ATOM	2136	CD2	PHE	268	15.081	36.303	59.682	1.00	18.13	AAAA
ATOM	2137	CE1	PHE	268	17.331	34.904	60.581	1.00	14.81	AAAA
ATOM	2138	CE2	PHE	268	15.027	34.900	59.849	1.00	17.45	AAAA
ATOM	2139	CZ	PHE	268	16.144	34.208	60.296	1.00	16.01	AAAA
ATOM	2140	C	PHE	268	15.179	40.699	59.510	1.00	18.33	AAAA
ATOM	2141	O	PHE	268	15.733	41.371	58.644	1.00	18.28	AAAA
ATOM	2142	N	ASN	269	14.679	41.236	60.613	1.00	21.04	AAAA
ATOM	2143	CA	ASN	269	14.763	42.675	60.859	1.00	22.89	AAAA
ATOM	2144	CB	ASN	269	13.365	43.298	60.940	1.00	20.55	AAAA
ATOM	2145	CG	ASN	269	12.551	43.071	59.686	1.00	26.13	AAAA
ATOM	2146	OD1	ASN	269	13.060	43.192	58.571	1.00	29.17	AAAA
ATOM	2147	ND2	ASN	269	11.268	42.767	59.860	1.00	28.26	AAAA
ATOM	2148	C	ASN	269	15.493	42.967	62.159	1.00	19.00	AAAA
ATOM	2149	O	ASN	269	14.984	43.683	63.019	1.00	21.85	AAAA
ATOM	2150	N	LEU	270	16.695	42.435	62.298	1.00	17.71	AAAA
ATOM	2151	CA	LEU	270	17.441	42.642	63.521	1.00	18.57	AAAA
ATOM	2152	CB	LEU	270	18.441	41.507	63.712	1.00	18.95	AAAA
ATOM	2153	CG	LEU	270	17.945	40.058	63.631	1.00	20.54	AAAA
ATOM	2154	CD1	LEU	270	19.070	39.174	64.152	1.00	14.19	AAAA
ATOM	2155	CD2	LEU	270	16.679	39.853	64.465	1.00	19.05	AAAA
ATOM	2156	C	LEU	270	18.203	43.971	63.583	1.00	22.83	AAAA
ATOM	2157	O	LEU	270	18.409	44.643	62.560	1.00	18.25	AAAA
ATOM	2158	N	SER	271	18.621	44.318	64.799	1.00	20.95	AAAA
ATOM	2159	CA	SER	271	19.414	45.518	65.081	1.00	18.28	AAAA
ATOM	2160	CB	SER	271	18.985	46.150	66.409	1.00	18.73	AAAA
ATOM	2161	OG	SER	271	19.347	45.327	67.512	1.00	22.28	AAAA
ATOM	2162	C	SER	271	20.875	45.073	65.224	1.00	19.98	AAAA
ATOM	2163	O	SER	271	21.122	43.899	65.537	1.00	18.82	AAAA
ATOM	2164	N	ASN	272	21.828	45.994	65.020	1.00	16.17	AAAA
ATOM	2165	CA	ASN	272	23.270	45.695	65.145	1.00	20.70	AAAA
ATOM	2166	CB	ASN	272	24.176	46.903	64.884	1.00	37.49	AAAA
ATOM	2167	CG	ASN	272	24.161	47.378	63.483	1.00	54.53	AAAA
ATOM	2168	OD1	ASN	272	24.702	48.454	63.199	1.00	45.61	AAAA
ATOM	2169	ND2	ASN	272	23.576	46.594	62.579	1.00	60.55	AAAA
ATOM	2170	C	ASN	272	23.586	45.343	66.580	1.00	18.03	AAAA
ATOM	2171	O	ASN	272	24.545	44.625	66.854	1.00	18.58	AAAA
ATOM	2172	N	VAL	273	22.831	45.938	67.500	1.00	19.57	AAAA
ATOM	2173	CA	VAL	273	23.053	45.698	68.919	1.00	22.12	AAAA
ATOM	2174	CB	VAL	273	22.345	46.765	69.765	1.00	26.91	AAAA
ATOM	2175	CG1	VAL	273	22.440	46.421	71.233	1.00	39.69	AAAA
ATOM	2176	CG2	VAL	273	23.034	48.115	69.531	1.00	34.73	AAAA
ATOM	2177	C	VAL	273	22.636	44.295	69.341	1.00	22.06	AAAA
ATOM	2178	O	VAL	273	23.249	43.708	70.217	1.00	16.89	AAAA

Figure 16-34

ATOM	2179	N	ALA	274	21.601	43.747	68.713	1.00	21.79	AAAA
ATOM	2180	CA	ALA	274	21.207	42.383	69.035	1.00	21.31	AAAA
ATOM	2181	CB	ALA	274	19.806	42.092	68.475	1.00	18.95	AAAA
ATOM	2182	C	ALA	274	22.259	41.451	68.400	1.00	17.83	AAAA
ATOM	2183	O	ALA	274	22.569	40.389	68.947	1.00	20.38	AAAA
ATOM	2184	N	PHE	275	22.798	41.859	67.245	1.00	16.01	AAAA
ATOM	2185	CA	PHE	275	23.828	41.089	66.536	1.00	16.46	AAAA
ATOM	2186	CB	PHE	275	24.220	41.835	65.253	1.00	24.56	AAAA
ATOM	2187	CG	PHE	275	25.363	41.222	64.492	1.00	23.01	AAAA
ATOM	2188	CD1	PHE	275	25.209	40.035	63.788	1.00	23.88	AAAA
ATOM	2189	CD2	PHE	275	26.590	41.877	64.443	1.00	22.40	AAAA
ATOM	2190	CE1	PHE	275	26.266	39.510	63.038	1.00	28.74	AAAA
ATOM	2191	CE2	PHE	275	27.654	41.365	63.700	1.00	35.03	AAAA
ATOM	2192	CZ	PHE	275	27.489	40.181	62.996	1.00	24.63	AAAA
ATOM	2193	C	PHE	275	25.030	40.964	67.469	1.00	25.06	AAAA
ATOM	2194	O	PHE	275	25.619	39.888	67.632	1.00	19.71	AAAA
ATOM	2195	N	LEU	276	25.366	42.080	68.101	1.00	17.49	AAAA
ATOM	2196	CA	LEU	276	26.482	42.139	69.030	1.00	24.23	AAAA
ATOM	2197	CB	LEU	276	26.736	43.606	69.416	1.00	20.44	AAAA
ATOM	2198	CG	LEU	276	28.001	43.967	70.211	1.00	39.65	AAAA
ATOM	2199	CD1	LEU	276	27.948	45.447	70.589	1.00	29.65	AAAA
ATOM	2200	CD2	LEU	276	28.102	43.143	71.460	1.00	32.41	AAAA
ATOM	2201	C	LEU	276	26.180	41.278	70.262	1.00	18.86	AAAA
ATOM	2202	O	LEU	276	27.045	40.529	70.727	1.00	17.99	AAAA
ATOM	2203	N	LYS	277	24.968	41.374	70.805	1.00	19.67	AAAA
ATOM	2204	CA	LYS	277	24.644	40.552	71.964	1.00	21.33	AAAA
ATOM	2205	CB	LYS	277	23.265	40.888	72.532	1.00	23.84	AAAA
ATOM	2206	CG	LYS	277	23.247	42.126	73.366	1.00	40.87	AAAA
ATOM	2207	CD	LYS	277	22.069	42.086	74.325	1.00	54.73	AAAA
ATOM	2208	CE	LYS	277	22.172	40.884	75.254	1.00	58.85	AAAA
ATOM	2209	NZ	LYS	277	21.051	40.844	76.228	1.00	55.34	AAAA
ATOM	2210	C	LYS	277	24.695	39.068	71.660	1.00	22.12	AAAA
ATOM	2211	O	LYS	277	25.074	38.264	72.513	1.00	22.19	AAAA
ATOM	2212	N	ALA	278	24.311	38.700	70.441	1.00	20.23	AAAA
ATOM	2213	CA	ALA	278	24.325	37.291	70.039	1.00	17.06	AAAA
ATOM	2214	CB	ALA	278	23.798	37.154	68.589	1.00	19.27	AAAA
ATOM	2215	C	ALA	278	25.760	36.767	70.127	1.00	16.94	AAAA
ATOM	2216	O	ALA	278	26.035	35.676	70.648	1.00	14.93	AAAA
ATOM	2217	N	PHE	279	26.679	37.564	69.606	1.00	18.88	AAAA
ATOM	2218	CA	PHE	279	28.099	37.231	69.626	1.00	21.01	AAAA
ATOM	2219	CB	PHE	279	28.880	38.392	68.998	1.00	16.79	AAAA
ATOM	2220	CG	PHE	279	30.370	38.264	69.120	1.00	20.23	AAAA
ATOM	2221	CD1	PHE	279	31.062	37.272	68.423	1.00	21.61	AAAA
ATOM	2222	CD2	PHE	279	31.088	39.159	69.905	1.00	23.24	AAAA
ATOM	2223	CE1	PHE	279	32.461	37.185	68.509	1.00	30.98	AAAA
ATOM	2224	CE2	PHE	279	32.480	39.081	69.995	1.00	24.82	AAAA
ATOM	2225	CZ	PHE	279	33.169	38.095	69.295	1.00	30.27	AAAA
ATOM	2226	C	PHE	279	28.576	36.995	71.067	1.00	25.48	AAAA
ATOM	2227	O	PHE	279	29.275	36.016	71.362	1.00	16.30	AAAA
ATOM	2228	N	ASN	280	28.194	37.898	71.962	1.00	22.30	AAAA
ATOM	2229	CA	ASN	280	28.599	37.777	73.352	1.00	24.49	AAAA
ATOM	2230	CB	ASN	280	28.391	39.109	74.080	1.00	27.17	AAAA
ATOM	2231	CG	ASN	280	29.344	40.183	73.578	1.00	20.88	AAAA
ATOM	2232	OD1	ASN	280	30.503	39.897	73.273	1.00	22.95	AAAA
ATOM	2233	ND2	ASN	280	28.875	41.421	73.522	1.00	27.85	AAAA
ATOM	2234	C	ASN	280	27.928	36.636	74.095	1.00	23.01	AAAA
ATOM	2235	O	ASN	280	28.510	36.062	75.016	1.00	21.91	AAAA
ATOM	2236	N	ILE	281	26.711	36.300	73.689	1.00	18.74	AAAA
ATOM	2237	CA	ILE	281	26.005	35.179	74.294	1.00	18.37	AAAA
ATOM	2238	CB	ILE	281	24.566	35.067	73.758	1.00	19.31	AAAA
ATOM	2239	CG2	ILE	281	23.977	33.725	74.135	1.00	28.87	AAAA
ATOM	2240	CG1	ILE	281	23.710	36.206	74.308	1.00	23.51	AAAA
ATOM	2241	CD1	ILE	281	22.279	36.193	73.776	1.00	26.47	AAAA
ATOM	2242	C	ILE	281	26.743	33.876	73.965	1.00	18.54	AAAA
ATOM	2243	O	ILE	281	26.830	32.973	74.801	1.00	19.69	AAAA
ATOM	2244	N	VAL	282	27.258	33.765	72.744	1.00	17.72	AAAA

53/263
Figure 16-35

ATOM	2245	CA	VAL	282	27.976	32.553	72.352	1.00	14.89	AAAA
ATOM	2246	CB	VAL	282	28.359	32.565	70.852	1.00	18.50	AAAA
ATOM	2247	CG1	VAL	282	29.342	31.440	70.567	1.00	20.73	AAAA
ATOM	2248	CG2	VAL	282	27.105	32.363	69.994	1.00	17.49	AAAA
ATOM	2249	C	VAL	282	29.241	32.433	73.198	1.00	21.79	AAAA
ATOM	2250	O	VAL	282	29.568	31.360	73.715	1.00	25.80	AAAA
ATOM	2251	N	ARG	283	29.935	33.549	73.361	1.00	19.14	AAAA
ATOM	2252	CA	ARG	283	31.161	33.548	74.150	1.00	23.51	AAAA
ATOM	2253	CB	ARG	283	31.851	34.898	74.023	1.00	20.64	AAAA
ATOM	2254	CG	ARG	283	32.338	35.200	72.607	1.00	19.65	AAAA
ATOM	2255	CD	ARG	283	32.754	36.645	72.474	1.00	25.70	AAAA
ATOM	2256	NE	ARG	283	33.970	36.944	73.215	1.00	36.05	AAAA
ATOM	2257	CZ	ARG	283	34.277	38.147	73.681	1.00	34.61	AAAA
ATOM	2258	NH1	ARG	283	33.448	39.169	73.488	1.00	35.23	AAAA
ATOM	2259	NH2	ARG	283	35.419	38.332	74.326	1.00	29.30	AAAA
ATOM	2260	C	ARG	283	30.911	33.219	75.622	1.00	25.44	AAAA
ATOM	2261	O	ARG	283	31.754	32.600	76.272	1.00	23.12	AAAA
ATOM	2262	N	GLU	284	29.765	33.632	76.151	1.00	26.79	AAAA
ATOM	2263	CA	GLU	284	29.462	33.338	77.553	1.00	31.77	AAAA
ATOM	2264	CB	GLU	284	28.243	34.115	78.033	1.00	30.96	AAAA
ATOM	2265	CG	GLU	284	28.399	35.605	77.957	1.00	50.56	AAAA
ATOM	2266	CD	GLU	284	27.137	36.320	78.365	1.00	63.75	AAAA
ATOM	2267	OE1	GLU	284	26.085	36.067	77.738	1.00	68.93	AAAA
ATOM	2268	OE2	GLU	284	27.198	37.133	79.309	1.00	72.01	AAAA
ATOM	2269	C	GLU	284	29.181	31.862	77.733	1.00	31.57	AAAA
ATOM	2270	O	GLU	284	29.410	31.310	78.803	1.00	33.08	AAAA
ATOM	2271	N	VAL	285	28.673	31.221	76.686	1.00	23.37	AAAA
ATOM	2272	CA	VAL	285	28.354	29.807	76.774	1.00	23.25	AAAA
ATOM	2273	CB	VAL	285	27.221	29.407	75.789	1.00	24.77	AAAA
ATOM	2274	CG1	VAL	285	26.952	27.913	75.881	1.00	26.98	AAAA
ATOM	2275	CG2	VAL	285	25.940	30.181	76.107	1.00	24.98	AAAA
ATOM	2276	C	VAL	285	29.567	28.942	76.479	1.00	31.41	AAAA
ATOM	2277	O	VAL	285	29.833	27.983	77.195	1.00	25.34	AAAA
ATOM	2278	N	PHE	286	30.316	29.276	75.431	1.00	27.27	AAAA
ATOM	2279	CA	PHE	286	31.463	28.457	75.086	1.00	22.47	AAAA
ATOM	2280	CB	PHE	286	31.289	27.904	73.667	1.00	22.26	AAAA
ATOM	2281	CG	PHE	286	30.168	26.918	73.536	1.00	25.71	AAAA
ATOM	2282	CD1	PHE	286	28.971	27.274	72.917	1.00	22.88	AAAA
ATOM	2283	CD2	PHE	286	30.294	25.631	74.069	1.00	24.49	AAAA
ATOM	2284	CE1	PHE	286	27.919	26.365	72.829	1.00	19.85	AAAA
ATOM	2285	CE2	PHE	286	29.246	24.714	73.987	1.00	27.48	AAAA
ATOM	2286	CZ	PHE	286	28.056	25.081	73.367	1.00	24.59	AAAA
ATOM	2287	C	PHE	286	32.854	29.059	75.225	1.00	21.53	AAAA
ATOM	2288	O	PHE	286	33.849	28.417	74.873	1.00	27.12	AAAA
ATOM	2289	N	GLY	287	32.937	30.272	75.754	1.00	23.76	AAAA
ATOM	2290	CA	GLY	287	34.237	30.896	75.901	1.00	24.17	AAAA
ATOM	2291	C	GLY	287	34.705	31.419	74.562	1.00	27.05	AAAA
ATOM	2292	O	GLY	287	33.888	31.670	73.667	1.00	18.06	AAAA
ATOM	2293	N	GLU	288	36.017	31.576	74.414	1.00	23.21	AAAA
ATOM	2294	CA	GLU	288	36.583	32.085	73.170	1.00	24.87	AAAA
ATOM	2295	CB	GLU	288	37.968	32.682	73.410	1.00	29.25	AAAA
ATOM	2296	CG	GLU	288	37.984	33.933	74.291	1.00	42.63	AAAA
ATOM	2297	CD	GLU	288	37.114	35.052	73.745	1.00	43.77	AAAA
ATOM	2298	OE1	GLU	288	37.235	35.380	72.544	1.00	36.82	AAAA
ATOM	2299	OE2	GLU	288	36.317	35.617	74.521	1.00	51.56	AAAA
ATOM	2300	C	GLU	288	36.693	31.028	72.072	1.00	20.85	AAAA
ATOM	2301	O	GLU	288	36.995	29.856	72.332	1.00	18.10	AAAA
ATOM	2302	N	GLY	289	36.447	31.468	70.843	1.00	26.12	AAAA
ATOM	2303	CA	GLY	289	36.517	30.588	69.692	1.00	20.71	AAAA
ATOM	2304	C	GLY	289	37.126	31.318	68.510	1.00	18.56	AAAA
ATOM	2305	O	GLY	289	37.669	32.404	68.679	1.00	16.59	AAAA
ATOM	2306	N	VAL	290	37.032	30.724	67.322	1.00	19.86	AAAA
ATOM	2307	CA	VAL	290	37.572	31.312	66.103	1.00	19.70	AAAA
ATOM	2308	CB	VAL	290	38.150	30.192	65.184	1.00	19.04	AAAA
ATOM	2309	CG1	VAL	290	38.667	30.769	63.853	1.00	15.54	AAAA
ATOM	2310	CG2	VAL	290	39.296	29.483	65.920	1.00	20.40	AAAA

ATOM	2311	C	VAL	290	36.408	32.040	65.427	1.00	20.90	AAAA
ATOM	2312	O	VAL	290	35.351	31.439	65.193	1.00	19.33	AAAA
ATOM	2313	N	TYR	291	36.598	33.325	65.125	1.00	15.37	AAAA
ATOM	2314	CA	TYR	291	35.543	34.140	64.524	1.00	16.79	AAAA
ATOM	2315	CB	TYR	291	35.412	35.438	65.317	1.00	16.42	AAAA
ATOM	2316	CG	TYR	291	35.375	35.181	66.808	1.00	18.60	AAAA
ATOM	2317	CD1	TYR	291	36.366	35.688	67.659	1.00	21.77	AAAA
ATOM	2318	CE1	TYR	291	36.368	35.385	69.030	1.00	22.55	AAAA
ATOM	2319	CD2	TYR	291	34.388	34.374	67.361	1.00	17.34	AAAA
ATOM	2320	CE2	TYR	291	34.381	34.066	68.718	1.00	20.24	AAAA
ATOM	2321	CZ	TYR	291	35.367	34.568	69.545	1.00	25.85	AAAA
ATOM	2322	OH	TYR	291	35.338	34.246	70.885	1.00	25.57	AAAA
ATOM	2323	C	TYR	291	35.720	34.446	63.031	1.00	14.97	AAAA
ATOM	2324	O	TYR	291	36.773	34.921	62.586	1.00	15.21	AAAA
ATOM	2325	N	LEU	292	34.660	34.189	62.273	1.00	14.06	AAAA
ATOM	2326	CA	LEU	292	34.674	34.392	60.824	1.00	15.03	AAAA
ATOM	2327	CB	LEU	292	34.461	33.046	60.108	1.00	13.66	AAAA
ATOM	2328	CG	LEU	292	35.342	21.856	60.496	1.00	19.04	AAAA
ATOM	2329	CD1	LEU	292	34.909	30.615	59.665	1.00	15.17	AAAA
ATOM	2330	CD2	LEU	292	36.792	32.190	60.252	1.00	19.18	AAAA
ATOM	2331	C	LEU	292	33.564	35.327	60.396	1.00	16.62	AAAA
ATOM	2332	O	LEU	292	32.575	35.488	61.107	1.00	14.76	AAAA
ATOM	2333	N	GLY	293	33.724	35.932	59.216	1.00	18.62	AAAA
ATOM	2334	CA	GLY	293	32.696	36.816	58.699	1.00	17.10	AAAA
ATOM	2335	C	GLY	293	31.611	35.954	58.068	1.00	23.44	AAAA
ATOM	2336	O	GLY	293	31.407	34.798	58.459	1.00	23.60	AAAA
ATOM	2337	N	GLY	294	30.915	36.501	57.085	1.00	24.96	AAAA
ATOM	2338	CA	GLY	294	29.871	35.738	56.434	1.00	27.07	AAAA
ATOM	2339	C	GLY	294	29.132	36.632	55.474	1.00	28.41	AAAA
ATOM	2340	O	GLY	294	29.605	37.722	55.167	1.00	25.66	AAAA
ATOM	2341	N	GLY	295	27.972	36.168	55.011	1.00	20.33	AAAA
ATOM	2342	CA	GLY	295	27.164	36.936	54.085	1.00	20.14	AAAA
ATOM	2343	C	GLY	295	26.742	38.244	54.730	1.00	25.34	AAAA
ATOM	2344	O	GLY	295	26.550	38.317	55.942	1.00	28.89	AAAA
ATOM	2345	N	GLY	296	26.614	39.274	53.909	1.00	28.52	AAAA
ATOM	2346	CA	GLY	296	26.230	40.598	54.367	1.00	23.21	AAAA
ATOM	2347	C	GLY	296	26.314	41.342	53.059	1.00	26.34	AAAA
ATOM	2348	O	GLY	296	27.359	41.324	52.414	1.00	26.05	AAAA
ATOM	2349	N	TYR	297	25.235	42.008	52.662	1.00	22.61	AAAA
ATOM	2350	CA	TYR	297	25.228	42.644	51.360	1.00	22.58	AAAA
ATOM	2351	CB	TYR	297	24.265	41.861	50.457	1.00	23.68	AAAA
ATOM	2352	CG	TYR	297	24.502	40.352	50.521	1.00	25.14	AAAA
ATOM	2353	CD1	TYR	297	23.981	39.571	51.568	1.00	28.31	AAAA
ATOM	2354	CE1	TYR	297	24.269	38.196	51.662	1.00	24.18	AAAA
ATOM	2355	CD2	TYR	297	25.307	39.725	49.577	1.00	29.74	AAAA
ATOM	2356	CE2	TYR	297	25.598	38.362	49.664	1.00	27.09	AAAA
ATOM	2357	CZ	TYR	297	25.085	37.606	50.696	1.00	28.68	AAAA
ATOM	2358	OH	TYR	297	25.407	36.261	50.739	1.00	28.17	AAAA
ATOM	2359	C	TYR	297	24.916	44.138	51.320	1.00	24.98	AAAA
ATOM	2360	O	TYR	297	24.841	44.714	50.237	1.00	26.51	AAAA
ATOM	2361	N	HIS	298	24.740	44.752	52.491	1.00	23.80	AAAA
ATOM	2362	CA	HIS	298	24.480	46.188	52.591	1.00	23.44	AAAA
ATOM	2363	CB	HIS	298	23.325	46.494	53.536	1.00	23.37	AAAA
ATOM	2364	CG	HIS	298	22.956	47.945	53.551	1.00	32.94	AAAA
ATOM	2365	CD2	HIS	298	23.491	48.983	54.232	1.00	24.31	AAAA
ATOM	2366	ND1	HIS	298	22.011	48.487	52.707	1.00	38.29	AAAA
ATOM	2367	CE1	HIS	298	21.978	49.797	52.868	1.00	26.60	AAAA
ATOM	2368	NE2	HIS	298	22.867	50.125	53.788	1.00	36.57	AAAA
ATOM	2369	C	HIS	298	25.757	46.775	53.184	1.00	23.11	AAAA
ATOM	2370	O	HIS	298	26.135	46.439	54.306	1.00	22.64	AAAA
ATOM	2371	N	PRO	299	26.430	47.673	52.445	1.00	21.07	AAAA
ATOM	2372	CD	PRO	299	26.078	48.207	51.117	1.00	27.42	AAAA
ATOM	2373	CA	PRO	299	27.676	48.286	52.910	1.00	26.62	AAAA
ATOM	2374	CB	PRO	299	28.041	49.228	51.755	1.00	28.95	AAAA
ATOM	2375	CG	PRO	299	26.678	49.600	51.196	1.00	35.16	AAAA
ATOM	2376	C	PRO	299	27.644	48.991	54.262	1.00	25.75	AAAA

55/263

Figure 16-37

ATOM	2377	O	PRO	299	28.565	48.845	55.068	1.00	24.36	AAAA
ATOM	2378	N	TYR	300	26.602	49.769	54.504	1.00	24.48	AAAA
ATOM	2379	CA	TYR	300	26.495	50.478	55.766	1.00	22.94	AAAA
ATOM	2380	CB	TYR	300	25.317	51.442	55.734	1.00	25.24	AAAA
ATOM	2381	CG	TYR	300	25.411	52.599	54.762	1.00	30.44	AAAA
ATOM	2382	CD1	TYR	300	26.366	52.634	53.746	1.00	26.01	AAAA
ATOM	2383	CE1	TYR	300	26.389	53.676	52.819	1.00	29.66	AAAA
ATOM	2384	CD2	TYR	300	24.490	53.640	54.827	1.00	31.37	AAAA
ATOM	2385	CE2	TYR	300	24.501	54.677	53.916	1.00	35.88	AAAA
ATOM	2386	CZ	TYR	300	25.448	54.689	52.913	1.00	38.44	AAAA
ATOM	2387	OH	TYR	300	25.417	55.700	51.990	1.00	33.41	AAAA
ATOM	2388	C	TYR	300	26.280	49.515	56.921	1.00	22.80	AAAA
ATOM	2389	O	TYR	300	26.895	49.643	57.983	1.00	19.14	AAAA
ATOM	2390	N	ALA	301	25.374	48.568	56.705	1.00	23.08	AAAA
ATOM	2391	CA	ALA	301	25.009	47.589	57.719	1.00	21.68	AAAA
ATOM	2392	CB	ALA	301	23.893	46.687	57.198	1.00	19.52	AAAA
ATOM	2393	C	ALA	301	26.216	46.762	58.098	1.00	23.49	AAAA
ATOM	2394	O	ALA	301	26.507	46.570	59.274	1.00	21.21	AAAA
ATOM	2395	N	LEU	302	26.904	46.275	57.072	1.00	23.19	AAAA
ATOM	2396	CA	LEU	302	28.090	45.463	57.234	1.00	20.66	AAAA
ATOM	2397	CB	LEU	302	28.602	45.057	55.844	1.00	23.31	AAAA
ATOM	2398	CG	LEU	302	29.932	44.335	55.611	1.00	36.66	AAAA
ATOM	2399	CD1	LEU	302	29.979	43.849	54.170	1.00	38.41	AAAA
ATOM	2400	CD2	LEU	302	31.104	45.255	55.879	1.00	28.52	AAAA
ATOM	2401	C	LEU	302	29.165	46.204	58.012	1.00	22.08	AAAA
ATOM	2402	O	LEU	302	29.653	45.713	59.020	1.00	20.43	AAAA
ATOM	2403	N	ALA	303	29.517	47.401	57.549	1.00	19.58	AAAA
ATOM	2404	CA	ALA	303	30.567	48.173	58.197	1.00	19.77	AAAA
ATOM	2405	CB	ALA	303	30.816	49.460	57.432	1.00	21.69	AAAA
ATOM	2406	C	ALA	303	30.324	48.485	59.657	1.00	19.19	AAAA
ATOM	2407	O	ALA	303	31.216	48.310	60.489	1.00	22.51	AAAA
ATOM	2408	N	ARG	304	29.128	48.954	59.993	1.00	20.12	AAAA
ATOM	2409	CA	ARG	304	28.872	49.296	61.377	1.00	18.04	AAAA
ATOM	2410	CB	ARG	304	27.566	50.114	61.511	1.00	21.09	AAAA
ATOM	2411	CG	ARG	304	27.532	51.481	60.792	1.00	24.34	AAAA
ATOM	2412	CD	ARG	304	26.259	52.259	61.206	1.00	27.09	AAAA
ATOM	2413	NE	ARG	304	25.090	51.398	61.116	1.00	45.73	AAAA
ATOM	2414	CZ	ARG	304	23.965	51.549	61.808	1.00	39.82	AAAA
ATOM	2415	NH1	ARG	304	23.813	52.550	62.677	1.00	28.40	AAAA
ATOM	2416	NH2	ARG	304	22.991	50.667	61.647	1.00	41.77	AAAA
ATOM	2417	C	ARG	304	28.794	48.073	62.280	1.00	21.00	AAAA
ATOM	2418	O	ARG	304	29.313	48.087	63.397	1.00	19.45	AAAA
ATOM	2419	N	ALA	305	28.159	47.008	61.796	1.00	19.93	AAAA
ATOM	2420	CA	ALA	305	28.002	45.809	62.610	1.00	18.70	AAAA
ATOM	2421	CB	ALA	305	26.998	44.830	61.933	1.00	18.26	AAAA
ATOM	2422	C	ALA	305	29.311	45.109	62.915	1.00	16.46	AAAA
ATOM	2423	O	ALA	305	29.564	44.736	64.061	1.00	19.49	AAAA
ATOM	2424	N	TRP	306	30.152	44.909	61.905	1.00	11.92	AAAA
ATOM	2425	CA	TRP	306	31.423	44.268	62.183	1.00	18.99	AAAA
ATOM	2426	CB	TRP	306	32.151	43.865	60.902	1.00	17.96	AAAA
ATOM	2427	CG	TRP	306	31.632	42.564	60.333	1.00	21.34	AAAA
ATOM	2428	CD2	TRP	306	31.852	42.058	59.014	1.00	16.55	AAAA
ATOM	2429	CE2	TRP	306	31.243	40.785	58.949	1.00	19.37	AAAA
ATOM	2430	CE3	TRP	306	32.507	42.556	57.878	1.00	17.80	AAAA
ATOM	2431	CD1	TRP	306	30.919	41.610	60.995	1.00	19.88	AAAA
ATOM	2432	NE1	TRP	306	30.680	40.535	60.170	1.00	15.95	AAAA
ATOM	2433	CZ2	TRP	306	31.270	40.002	57.787	1.00	24.85	AAAA
ATOM	2434	CZ3	TRP	306	32.534	41.781	56.725	1.00	29.69	AAAA
ATOM	2435	CH2	TRP	306	31.917	40.513	56.691	1.00	17.04	AAAA
ATOM	2436	C	TRP	306	32.289	45.168	63.018	1.00	20.26	AAAA
ATOM	2437	O	TRP	306	33.159	44.726	63.752	1.00	21.20	AAAA
ATOM	2438	N	THR	307	32.061	46.491	62.911	1.00	18.60	AAAA
ATOM	2439	CA	THR	307	32.843	47.412	63.722	1.00	16.88	AAAA
ATOM	2440	CB	THR	307	32.579	48.885	63.312	1.00	22.05	AAAA
ATOM	2441	OG1	THR	307	33.218	49.132	62.051	1.00	21.58	AAAA
ATOM	2442	CG2	THR	307	33.126	49.857	64.356	1.00	24.86	AAAA

Figure 16-38

ATOM	2443	C	THR	307	32.493	47.146	65.187	1.00	17.47	AAAA
ATOM	2444	O	THR	307	33.377	47.142	66.039	1.00	18.94	AAAA
ATOM	2445	N	LEU	308	31.216	46.901	65.487	1.00	19.97	AAAA
ATOM	2446	CA	LEU	308	30.834	46.587	66.866	1.00	22.54	AAAA
ATOM	2447	CB	LEU	308	29.318	46.365	66.989	1.00	21.13	AAAA
ATOM	2448	CG	LEU	308	28.415	47.579	66.751	1.00	22.82	AAAA
ATOM	2449	CD1	LEU	308	26.937	47.219	67.023	1.00	25.01	AAAA
ATOM	2450	CD2	LEU	308	28.870	48.710	67.685	1.00	29.09	AAAA
ATOM	2451	C	LEU	308	31.578	45.331	67.336	1.00	22.98	AAAA
ATOM	2452	O	LEU	308	32.056	45.250	68.479	1.00	22.27	AAAA
ATOM	2453	N	ILE	309	31.677	44.342	66.454	1.00	22.54	AAAA
ATOM	2454	CA	ILE	309	32.377	43.114	66.801	1.00	17.09	AAAA
ATOM	2455	CB	ILE	309	32.318	42.073	65.664	1.00	18.12	AAAA
ATOM	2456	CG2	ILE	309	33.170	40.870	66.033	1.00	24.16	AAAA
ATOM	2457	CG1	ILE	309	30.871	41.655	65.399	1.00	18.26	AAAA
ATOM	2458	CD1	ILE	309	30.205	40.989	66.586	1.00	26.57	AAAA
ATOM	2459	C	ILE	309	33.849	43.410	67.067	1.00	20.84	AAAA
ATOM	2460	O	ILE	309	34.426	42.905	68.031	1.00	25.20	AAAA
ATOM	2461	N	TRP	310	34.466	44.223	66.214	1.00	16.86	AAAA
ATOM	2462	CA	TRP	310	35.888	44.517	66.411	1.00	17.86	AAAA
ATOM	2463	CB	TRP	310	36.439	45.319	65.235	1.00	14.83	AAAA
ATOM	2464	CG	TRP	310	37.879	45.648	65.397	1.00	16.63	AAAA
ATOM	2465	CD2	TRP	310	38.967	44.718	65.560	1.00	18.62	AAAA
ATOM	2466	CE2	TRP	310	40.131	45.478	65.799	1.00	25.60	AAAA
ATOM	2467	CE3	TRP	310	39.069	43.319	65.529	1.00	24.06	AAAA
ATOM	2468	CD1	TRP	310	38.418	46.895	65.533	1.00	19.82	AAAA
ATOM	2469	NE1	TRP	310	39.768	46.801	65.777	1.00	25.84	AAAA
ATOM	2470	CZ2	TRP	310	41.383	44.887	66.006	1.00	26.14	AAAA
ATOM	2471	CZ3	TRP	310	40.308	42.730	65.735	1.00	24.89	AAAA
ATOM	2472	CH2	TRP	310	41.452	43.515	65.971	1.00	24.96	AAAA
ATOM	2473	C	TRP	310	36.112	45.263	67.733	1.00	20.86	AAAA
ATOM	2474	O	TRP	310	37.050	44.957	68.478	1.00	21.38	AAAA
ATOM	2475	N	CYS	311	35.242	46.226	68.030	1.00	24.22	AAAA
ATOM	2476	CA	CYS	311	35.349	46.971	69.280	1.00	27.66	AAAA
ATOM	2477	CB	CYS	311	34.297	48.097	69.343	1.00	25.37	AAAA
ATOM	2478	SG	CYS	311	34.618	49.528	68.253	1.00	27.22	AAAA
ATOM	2479	C	CYS	311	35.224	46.042	70.490	1.00	22.95	AAAA
ATOM	2480	O	CYS	311	35.986	46.180	71.441	1.00	25.47	AAAA
ATOM	2481	N	GLU	312	34.284	45.089	70.457	1.00	17.03	AAAA
ATOM	2482	CA	GLU	312	34.120	44.129	71.569	1.00	22.44	AAAA
ATOM	2483	CB	GLU	312	33.011	43.110	71.280	1.00	20.81	AAAA
ATOM	2484	CG	GLU	312	31.856	43.048	72.258	1.00	43.65	AAAA
ATOM	2485	CD	GLU	312	32.265	42.971	73.717	1.00	29.63	AAAA
ATOM	2486	OE1	GLU	312	33.022	42.059	74.119	1.00	38.85	AAAA
ATOM	2487	OE2	GLU	312	31.804	43.844	74.473	1.00	53.22	AAAA
ATOM	2488	C	GLU	312	35.395	43.309	71.778	1.00	27.47	AAAA
ATOM	2489	O	GLU	312	35.899	43.178	72.895	1.00	22.33	AAAA
ATOM	2490	N	LEU	313	35.899	42.723	70.696	1.00	23.82	AAAA
ATOM	2491	CA	LEU	313	37.101	41.889	70.771	1.00	20.72	AAAA
ATOM	2492	CB	LEU	313	37.380	41.222	69.422	1.00	27.82	AAAA
ATOM	2493	CG	LEU	313	36.403	40.167	68.903	1.00	33.55	AAAA
ATOM	2494	CD1	LEU	313	36.839	39.738	67.512	1.00	24.03	AAAA
ATOM	2495	CD2	LEU	313	36.379	38.981	69.846	1.00	28.20	AAAA
ATOM	2496	C	LEU	313	38.343	42.670	71.181	1.00	18.21	AAAA
ATOM	2497	O	LEU	313	39.119	42.205	72.017	1.00	21.48	AAAA
ATOM	2498	N	SER	314	38.492	43.848	70.580	1.00	19.41	AAAA
ATOM	2499	CA	SER	314	39.627	44.753	70.775	1.00	28.26	AAAA
ATOM	2500	CB	SER	314	39.625	45.821	69.663	1.00	22.55	AAAA
ATOM	2501	OG	SER	314	40.732	46.696	69.759	1.00	61.92	AAAA
ATOM	2502	C	SER	314	39.619	45.429	72.144	1.00	30.18	AAAA
ATOM	2503	O	SER	314	40.631	45.969	72.590	1.00	25.04	AAAA
ATOM	2504	N	GLY	315	38.477	45.407	72.806	1.00	28.04	AAAA
ATOM	2505	CA	GLY	315	38.393	46.009	74.119	1.00	33.84	AAAA
ATOM	2506	C	GLY	315	38.324	47.518	74.105	1.00	36.93	AAAA
ATOM	2507	O	GLY	315	38.811	48.178	75.022	1.00	37.00	AAAA
ATOM	2508	N	ARG	316	37.739	48.090	73.065	1.00	31.33	AAAA

Figure 16-39

ATOM	2509	CA	ARG	316	37.631	49.536	73.042	1.00	39.10	AAAA
ATOM	2510	CB	ARG	316	38.347	50.108	71.830	1.00	45.15	AAAA
ATOM	2511	CG	ARG	316	37.722	49.834	70.501	1.00	46.02	AAAA
ATOM	2512	CD	ARG	316	38.620	50.459	69.449	1.00	44.83	AAAA
ATOM	2513	NE	ARG	316	39.898	49.767	69.357	1.00	37.91	AAAA
ATOM	2514	CZ	ARG	316	40.945	50.219	68.674	1.00	27.39	AAAA
ATOM	2515	NH1	ARG	316	40.854	51.371	68.034	1.00	50.24	AAAA
ATOM	2516	NH2	ARG	316	42.054	49.493	68.572	1.00	34.51	AAAA
ATOM	2517	C	ARG	316	36.179	49.984	73.058	1.00	35.43	AAAA
ATOM	2518	O	ARG	316	35.292	49.271	72.596	1.00	30.71	AAAA
ATOM	2519	N	GLU	317	35.931	51.162	73.612	1.00	34.06	AAAA
ATOM	2520	CA	GLU	317	34.569	51.663	73.671	1.00	37.96	AAAA
ATOM	2521	CB	GLU	317	34.481	52.914	74.552	1.00	43.60	AAAA
ATOM	2522	CG	GLU	317	33.961	52.630	75.960	1.00	60.36	AAAA
ATOM	2523	CD	GLU	317	34.768	51.575	76.701	1.00	70.70	AAAA
ATOM	2524	OE1	GLU	317	34.375	51.217	77.832	1.00	76.71	AAAA
ATOM	2525	OE2	GLU	317	35.793	51.104	76.162	1.00	78.36	AAAA
ATOM	2526	C	GLU	317	34.068	51.958	72.280	1.00	35.65	AAAA
ATOM	2527	O	GLU	317	34.843	52.322	71.390	1.00	32.91	AAAA
ATOM	2528	N	VAL	318	32.767	51.772	72.094	1.00	30.52	AAAA
ATOM	2529	CA	VAL	318	32.138	52.012	70.808	1.00	37.04	AAAA
ATOM	2530	CB	VAL	318	30.877	51.138	70.638	1.00	36.48	AAAA
ATOM	2531	CG1	VAL	318	30.278	51.366	69.268	1.00	40.43	AAAA
ATOM	2532	CG2	VAL	318	31.222	49.674	70.846	1.00	33.75	AAAA
ATOM	2533	C	VAL	318	31.719	53.465	70.737	1.00	28.96	AAAA
ATOM	2534	O	VAL	318	30.930	53.915	71.556	1.00	33.56	AAAA
ATOM	2535	N	PRO	319	32.258	54.229	69.773	1.00	29.20	AAAA
ATOM	2536	CD	PRO	319	33.243	53.924	68.726	1.00	31.62	AAAA
ATOM	2537	CA	PRO	319	31.858	55.637	69.684	1.00	28.99	AAAA
ATOM	2538	CB	PRO	319	32.709	56.154	68.528	1.00	32.17	AAAA
ATOM	2539	CG	PRO	319	32.850	54.926	67.664	1.00	41.36	AAAA
ATOM	2540	C	PRO	319	30.365	55.680	69.377	1.00	36.95	AAAA
ATOM	2541	O	PRO	319	29.847	54.795	68.695	1.00	32.86	AAAA
ATOM	2542	N	GLU	320	29.646	56.683	69.855	1.00	34.61	AAAA
ATOM	2543	CA	GLU	320	28.230	56.657	69.544	1.00	35.13	AAAA
ATOM	2544	CB	GLU	320	27.419	57.416	70.595	1.00	52.97	AAAA
ATOM	2545	CG	GLU	320	27.751	58.875	70.738	1.00	56.06	AAAA
ATOM	2546	CD	GLU	320	26.822	59.558	71.721	1.00	65.58	AAAA
ATOM	2547	OE1	GLU	320	25.604	59.619	71.444	1.00	64.27	AAAA
ATOM	2548	OE2	GLU	320	27.306	60.022	72.775	1.00	72.99	AAAA
ATOM	2549	C	GLU	320	27.943	57.192	68.153	1.00	35.13	AAAA
ATOM	2550	O	GLU	320	26.916	56.879	67.565	1.00	37.43	AAAA
ATOM	2551	N	LYS	321	28.880	57.953	67.604	1.00	28.22	AAAA
ATOM	2552	CA	LYS	321	28.700	58.555	66.289	1.00	36.58	AAAA
ATOM	2553	CB	LYS	321	28.666	60.071	66.454	1.00	44.87	AAAA
ATOM	2554	CG	LYS	321	29.987	60.606	67.023	1.00	55.73	AAA
ATOM	2555	CD	LYS	321	30.305	60.020	68.410	1.00	57.27	AAA
ATOM	2556	CE	LYS	321	31.733	60.310	68.840	1.00	54.59	AAA
ATOM	2557	NZ	LYS	321	32.024	61.774	68.848	1.00	67.47	AAAA
ATOM	2558	C	LYS	321	29.823	58.211	65.315	1.00	34.44	AAAA
ATOM	2559	O	LYS	321	30.912	57.818	65.731	1.00	33.83	AAAA
ATOM	2560	N	LEU	322	29.549	58.354	64.019	1.00	30.21	AAAA
ATOM	2561	CA	LEU	322	30.575	58.135	62.998	1.00	29.45	AAAA
ATOM	2562	CB	LEU	322	29.966	57.677	61.677	1.00	32.21	AAAA
ATOM	2563	CG	LEU	322	29.240	56.338	61.651	1.00	38.94	AAAA
ATOM	2564	CD1	LEU	322	29.008	55.977	60.186	1.00	38.44	AAAA
ATOM	2565	CD2	LEU	322	30.072	55.261	62.337	1.00	42.11	AAAA
ATOM	2566	C	LEU	322	31.228	59.503	62.783	1.00	33.28	AAAA
ATOM	2567	O	LEU	322	30.544	60.519	62.872	1.00	31.45	AAAA
ATOM	2568	N	ASN	323	32.533	59.539	62.519	1.00	34.38	AAAA
ATOM	2569	CA	ASN	323	33.208	60.824	62.294	1.00	36.53	AAAA
ATOM	2570	CB	ASN	323	34.701	60.737	62.600	1.00	42.85	AAA
ATOM	2571	CG	ASN	323	35.484	60.081	61.480	1.00	50.51	AAA
ATOM	2572	OD1	ASN	323	35.215	58.942	61.109	1.00	51.23	AAA
ATOM	2573	ND2	ASN	323	36.455	60.807	60.928	1.00	60.23	AAA
ATOM	2574	C	ASN	323	33.027	61.171	60.822	1.00	34.69	AAA

58/263

Figure 16-40

ATOM	2575	O	ASN	323	32.429	60.395	60.075	1.00	34.06	AAAA
ATOM	2576	N	ASN	324	33.551	62.317	60.390	1.00	23.73	AAAA
ATOM	2577	CA	ASN	324	33.385	62.720	58.995	1.00	31.06	AAAA
ATOM	2578	CB	ASN	324	33.868	64.155	58.784	1.00	36.07	AAAA
ATOM	2579	CG	ASN	324	32.974	65.163	59.450	1.00	45.77	AAAA
ATOM	2580	OD1	ASN	324	31.765	65.189	59.206	1.00	39.55	AAAA
ATOM	2581	ND2	ASN	324	33.555	66.008	60.291	1.00	39.12	AAAA
ATOM	2582	C	ASN	324	34.047	61.810	57.971	1.00	24.87	AAAA
ATOM	2583	O	ASN	324	33.451	61.483	56.941	1.00	31.91	AAAA
ATOM	2584	N	LYS	325	35.276	61.405	58.250	1.00	27.73	AAAA
ATOM	2585	CA	LYS	325	35.991	60.538	57.333	1.00	29.55	AAAA
ATOM	2586	CB	LYS	325	37.351	60.182	57.929	1.00	37.43	AAAA
ATOM	2587	CG	LYS	325	38.250	59.396	57.004	1.00	44.84	AAAA
ATOM	2588	CD	LYS	325	39.684	59.435	57.502	1.00	50.89	AAAA
ATOM	2589	CE	LYS	325	40.191	60.873	57.561	1.00	54.82	AAAA
ATOM	2590	NZ	LYS	325	41.621	60.980	57.969	1.00	65.70	AAAA
ATOM	2591	C	LYS	325	35.161	59.279	57.078	1.00	27.99	AAAA
ATOM	2592	O	LYS	325	35.016	58.836	55.938	1.00	31.80	AAAA
ATOM	2593	N	ALA	326	34.602	58.721	58.142	1.00	26.07	AAAA
ATOM	2594	CA	ALA	326	33.781	57.506	58.030	1.00	24.38	AAAA
ATOM	2595	CB	ALA	326	33.470	56.982	59.428	1.00	27.34	AAAA
ATOM	2596	C	ALA	326	32.478	57.709	57.231	1.00	25.78	AAAA
ATOM	2597	O	ALA	326	32.131	56.890	56.369	1.00	27.37	AAAA
ATOM	2598	N	LYS	327	31.749	58.790	57.496	1.00	27.31	AAAA
ATOM	2599	CA	LYS	327	30.502	59.027	56.758	1.00	28.56	AAAA
ATOM	2600	CB	LYS	327	29.759	60.251	57.313	1.00	28.67	AAAA
ATOM	2601	CG	LYS	327	29.491	60.209	58.812	1.00	36.72	AAAA
ATOM	2602	CD	LYS	327	28.643	61.407	59.255	1.00	40.34	AAAA
ATOM	2603	CE	LYS	327	28.645	61.594	60.769	1.00	38.91	AAAA
ATOM	2604	NZ	LYS	327	28.163	60.429	61.556	1.00	47.67	AAAA
ATOM	2605	C	LYS	327	30.792	59.244	55.269	1.00	29.15	AAAA
ATOM	2606	O	LYS	327	30.097	58.719	54.393	1.00	27.76	AAAA
ATOM	2607	N	GLU	328	31.829	60.015	54.972	1.00	31.59	AAAA
ATOM	2608	CA	GLU	328	32.167	60.265	53.581	1.00	28.93	AAAA
ATOM	2609	CB	GLU	328	33.257	61.332	53.515	1.00	32.30	AAAA
ATOM	2610	CG	GLU	328	32.745	62.652	54.067	1.00	47.50	AAAA
ATOM	2611	CD	GLU	328	33.764	63.772	54.032	1.00	46.67	AAAA
ATOM	2612	OE1	GLU	328	34.325	64.037	52.951	1.00	56.88	AAAA
ATOM	2613	OE2	GLU	328	33.984	64.402	55.087	1.00	42.24	AAAA
ATOM	2614	C	GLU	328	32.575	58.975	52.871	1.00	30.46	AAAA
ATOM	2615	O	GLU	328	32.226	58.753	51.704	1.00	26.29	AAAA
ATOM	2616	N	LEU	329	33.292	58.112	53.584	1.00	24.93	AAAA
ATOM	2617	CA	LEU	329	33.701	56.828	53.017	1.00	24.80	AAAA
ATOM	2618	CB	LEU	329	34.478	56.003	54.053	1.00	25.70	AAAA
ATOM	2619	CG	LEU	329	34.730	54.522	53.703	1.00	19.71	AAAA
ATOM	2620	CD1	LEU	329	33.569	54.413	52.430	1.00	25.26	AAAA
ATOM	2621	CD2	LEU	329	35.412	53.833	54.863	1.00	24.73	AAAA
ATOM	2622	C	LEU	329	32.443	56.059	52.603	1.00	23.50	AAAA
ATOM	2623	O	LEU	329	32.310	55.650	51.453	1.00	25.60	AAAA
ATOM	2624	N	LEU	330	31.516	55.881	53.539	1.00	23.02	AAAA
ATOM	2625	CA	LEU	330	30.289	55.145	53.242	1.00	23.85	AAAA
ATOM	2626	CB	LEU	330	29.414	55.030	54.484	1.00	21.74	AAAA
ATOM	2627	CG	LEU	330	30.039	54.252	55.642	1.00	25.29	AAAA
ATOM	2628	CD1	LEU	330	28.984	54.053	56.724	1.00	30.59	AAAA
ATOM	2629	CD2	LEU	330	30.538	52.905	55.168	1.00	22.44	AAAA
ATOM	2630	C	LEU	330	29.491	55.769	52.113	1.00	26.94	AAAA
ATOM	2631	O	LEU	330	28.968	55.060	51.252	1.00	26.65	AAAA
ATOM	2632	N	LYS	331	29.404	57.097	52.111	1.00	30.82	AAAA
ATOM	2633	CA	LYS	331	28.667	57.795	51.066	1.00	29.53	AAAA
ATOM	2634	CB	LYS	331	28.537	59.292	51.407	1.00	29.67	AAAA
ATOM	2635	CG	LYS	331	27.814	59.567	52.714	1.00	36.06	AAAA
ATOM	2636	CD	LYS	331	27.688	61.055	52.990	1.00	42.75	AAAA
ATOM	2637	CE	LYS	331	26.828	61.737	51.939	1.00	53.98	AAAA
ATOM	2638	NZ	LYS	331	26.634	63.185	52.234	1.00	67.57	AAAA
ATOM	2639	C	LYS	331	29.315	57.628	49.692	1.00	30.07	AAAA
ATOM	2640	O	LYS	331	28.634	57.759	48.672	1.00	36.20	AAAA

Figure 16-41

ATOM	2641	N	SER	332	30.608	57.305	49.657	1.00	30.08	AAAA
ATOM	2642	CA	SER	332	31.322	57.153	48.385	1.00	33.35	AAAA
ATOM	2643	CB	SER	332	32.834	57.312	48.590	1.00	40.36	AAAA
ATOM	2644	OG	SER	332	33.396	56.169	49.219	1.00	34.04	AAAA
ATOM	2645	C	SER	332	31.061	55.821	47.693	1.00	37.72	AAAA
ATOM	2646	O	SER	332	31.354	55.661	46.507	1.00	30.78	AAAA
ATOM	2647	N	ILE	333	30.521	54.865	48.440	1.00	30.61	AAAA
ATOM	2648	CA	ILE	333	30.219	53.547	47.899	1.00	37.59	AAAA
ATOM	2649	CB	ILE	333	29.901	52.551	49.022	1.00	33.59	AAAA
ATOM	2650	CG2	ILE	333	29.738	51.146	48.442	1.00	37.05	AAAA
ATOM	2651	CG1	ILE	333	31.015	52.564	50.065	1.00	38.95	AAAA
ATOM	2652	CD1	ILE	333	30.706	51.727	51.282	1.00	46.83	AAAA
ATOM	2653	C	ILE	333	28.990	53.620	46.998	1.00	43.41	AAAA
ATOM	2654	O	ILE	333	27.889	53.876	47.479	1.00	46.24	AAAA
ATOM	2655	N	ASP	334	29.158	53.423	45.696	1.00	47.97	AAAA
ATOM	2656	CA	ASP	334	27.976	53.447	44.847	1.00	53.47	AAAA
ATOM	2657	CB	ASP	334	28.333	53.535	43.358	1.00	61.52	AAAA
ATOM	2658	CG	ASP	334	29.223	52.406	42.897	1.00	64.75	AAAA
ATOM	2659	OD1	ASP	334	29.379	52.248	41.666	1.00	66.93	AAAA
ATOM	2660	OD2	ASP	334	29.779	51.691	43.758	1.00	65.93	AAAA
ATOM	2661	C	ASP	334	27.248	52.144	45.161	1.00	51.83	AAAA
ATOM	2662	O	ASP	334	27.626	51.067	44.699	1.00	46.80	AAAA
ATOM	2663	N	PHE	335	26.215	52.249	45.986	1.00	54.96	AAAA
ATOM	2664	CA	PHE	335	25.455	51.080	46.392	1.00	50.60	AAAA
ATOM	2665	CB	PHE	335	25.413	51.003	47.920	1.00	39.55	AAAA
ATOM	2666	CG	PHE	335	24.380	50.054	48.440	1.00	37.98	AAAA
ATOM	2667	CD1	PHE	335	24.389	48.715	48.054	1.00	46.72	AAAA
ATOM	2668	CD2	PHE	335	23.362	50.506	49.262	1.00	34.23	AAAA
ATOM	2669	CE1	PHE	335	23.389	47.842	48.478	1.00	49.80	AAAA
ATOM	2670	CE2	PHE	335	22.361	49.644	49.689	1.00	48.51	AAAA
ATOM	2671	CZ	PHE	335	22.373	48.309	49.296	1.00	40.44	AAAA
ATOM	2672	C	PHE	335	24.033	51.000	45.839	1.00	54.52	AAAA
ATOM	2673	O	PHE	335	23.603	49.939	45.379	1.00	59.24	AAAA
ATOM	2674	N	GLU	336	23.302	52.108	45.888	1.00	50.94	AAAA
ATOM	2675	CA	GLU	336	21.923	52.119	45.406	1.00	57.05	AAAA
ATOM	2676	CB	GLU	336	21.853	51.751	43.924	1.00	60.27	AAAA
ATOM	2677	CG	GLU	336	20.430	51.627	43.422	1.00	68.55	AAAA
ATOM	2678	CD	GLU	336	20.352	51.126	42.001	1.00	80.03	AAAA
ATOM	2679	OE1	GLU	336	20.860	50.013	41.735	1.00	84.64	AAAA
ATOM	2680	OE2	GLU	336	19.777	51.841	41.153	1.00	80.68	AAAA
ATOM	2681	C	GLU	336	21.065	51.135	46.201	1.00	55.73	AAAA
ATOM	2682	O	GLU	336	21.219	49.917	46.089	1.00	51.33	AAAA
ATOM	2683	N	GLU	337	20.151	51.679	46.992	1.00	49.54	AAAA
ATOM	2684	CA	GLU	337	19.267	50.880	47.821	1.00	48.19	AAAA
ATOM	2685	CB	GLU	337	18.510	51.822	48.764	1.00	47.73	AAAA
ATOM	2686	CG	GLU	337	18.084	51.205	50.077	1.00	55.69	AAAA
ATOM	2687	CD	GLU	337	19.269	50.720	50.904	1.00	50.17	AAAA
ATOM	2688	OE1	GLU	337	20.111	51.548	51.345	1.00	36.03	AAAA
ATOM	2689	OE2	GLU	337	19.358	49.494	51.105	1.00	51.25	AAAA
ATOM	2690	C	GLU	337	18.294	50.083	46.936	1.00	49.13	AAAA
ATOM	2691	O	GLU	337	17.816	50.588	45.916	1.00	48.61	AAAA
ATOM	2692	N	PHE	338	18.015	48.837	47.313	1.00	48.15	AAAA
ATOM	2693	CA	PHE	338	17.092	48.000	46.547	1.00	48.12	AAAA
ATOM	2694	CB	PHE	338	16.870	46.658	47.249	1.00	54.54	AAAA
ATOM	2695	CG	PHE	338	15.883	45.777	46.548	1.00	57.22	AAAA
ATOM	2696	CD1	PHE	338	16.115	45.366	45.243	1.00	60.01	AAAA
ATOM	2697	CD2	PHE	338	14.699	45.398	47.171	1.00	55.04	AAAA
ATOM	2698	CE1	PHE	338	15.185	44.597	44.566	1.00	60.84	AAAA
ATOM	2699	CE2	PHE	338	13.758	44.624	46.497	1.00	59.41	AAAA
ATOM	2700	CZ	PHE	338	14.002	44.224	45.189	1.00	57.18	AAAA
ATOM	2701	C	PHE	338	15.755	48.714	46.380	1.00	45.46	AAAA
ATOM	2702	O	PHE	338	15.274	48.900	45.263	1.00	51.11	AAAA
ATOM	2703	N	ASP	339	15.154	49.098	47.501	1.00	40.38	AAA
ATOM	2704	CA	ASP	339	13.890	49.820	47.488	1.00	49.97	AAA
ATOM	2705	CB	ASP	339	13.270	49.821	48.886	1.00	53.23	AAA
ATOM	2706	CG	ASP	339	12.000	50.659	48.968	1.00	57.40	AAA

Figure 16-42

ATOM	2707	OD1	ASP	339	12.039	51.858	48.616	1.00	53.79	AAAA
ATOM	2708	OD2	ASP	339	10.963	50.118	49.401	1.00	51.15	AAAA
ATOM	2709	C	ASP	339	14.215	51.248	47.076	1.00	55.06	AAAA
ATOM	2710	O	ASP	339	14.994	51.922	47.748	1.00	56.47	AAAA
ATOM	2711	N	ASP	340	13.623	51.708	45.978	1.00	58.46	AAAA
ATOM	2712	CA	ASP	340	13.874	53.059	45.484	1.00	67.72	AAAA
ATOM	2713	CB	ASP	340	12.683	53.559	44.664	1.00	71.52	AAAA
ATOM	2714	CG	ASP	340	12.611	52.913	43.295	1.00	79.72	AAAA
ATOM	2715	OD1	ASP	340	12.528	51.667	43.224	1.00	86.74	AAAA
ATOM	2716	OD2	ASP	340	12.640	53.655	42.288	1.00	83.40	AAAA
ATOM	2717	C	ASP	340	14.209	54.072	46.572	1.00	69.65	AAAA
ATOM	2718	O	ASP	340	15.204	54.794	46.463	1.00	70.13	AAAA
ATOM	2719	N	GLU	341	13.392	54.130	47.620	1.00	67.11	AAAA
ATOM	2720	CA	GLU	341	13.668	55.077	48.689	1.00	67.87	AAAA
ATOM	2721	CB	GLU	341	13.195	56.478	48.278	1.00	74.87	AAAA
ATOM	2722	CG	GLU	341	13.502	57.576	49.298	1.00	82.72	AAAA
ATOM	2723	CD	GLU	341	13.162	58.974	48.790	1.00	90.80	AAAA
ATOM	2724	OE1	GLU	341	11.988	59.215	48.431	1.00	90.38	AAAA
ATOM	2725	OE2	GLU	341	14.072	59.835	48.752	1.00	93.36	AAAA
ATOM	2726	C	GLU	341	13.101	54.719	50.058	1.00	60.22	AAAA
ATOM	2727	O	GLU	341	11.929	54.955	50.347	1.00	58.81	AAAA
ATOM	2728	N	VAL	342	13.956	54.144	50.897	1.00	57.28	AAAA
ATOM	2729	CA	VAL	342	13.594	53.781	52.262	1.00	52.09	AAAA
ATOM	2730	CB	VAL	342	14.195	52.419	52.669	1.00	53.17	AAAA
ATOM	2731	CG1	VAL	342	13.730	52.042	54.070	1.00	46.16	AAAA
ATOM	2732	CG2	VAL	342	13.815	51.356	51.663	1.00	59.09	AAAA
ATOM	2733	C	VAL	342	14.263	54.843	53.124	1.00	53.31	AAAA
ATOM	2734	O	VAL	342	13.763	55.230	54.185	1.00	57.79	AAAA
ATOM	2735	N	ASP	343	15.398	55.306	52.610	1.00	46.24	AAAA
ATOM	2736	CA	ASP	343	16.268	56.289	53.243	1.00	42.60	AAAA
ATOM	2737	CB	ASP	343	15.521	57.510	53.781	1.00	43.88	AAAA
ATOM	2738	CG	ASP	343	16.480	58.581	54.290	1.00	46.82	AAAA
ATOM	2739	OD1	ASP	343	16.028	59.581	54.887	1.00	46.16	AAAA
ATOM	2740	OD2	ASP	343	17.700	58.414	54.075	1.00	33.01	AAAA
ATOM	2741	C	ASP	343	17.012	55.636	54.395	1.00	35.45	AAAA
ATOM	2742	O	ASP	343	16.487	55.480	55.502	1.00	29.39	AAAA
ATOM	2743	N	ARG	344	18.247	55.249	54.124	1.00	30.51	AAAA
ATOM	2744	CA	ARG	344	19.059	54.613	55.140	1.00	29.43	AAAA
ATOM	2745	CB	ARG	344	19.736	53.377	54.561	1.00	30.10	AAAA
ATOM	2746	CG	ARG	344	18.803	52.258	54.180	1.00	33.95	AAAA
ATOM	2747	CD	ARG	344	17.981	51.770	55.365	1.00	20.92	AAAA
ATOM	2748	NE	ARG	344	17.120	50.673	54.936	1.00	29.72	AAAA
ATOM	2749	CZ	ARG	344	16.110	50.176	55.639	1.00	29.13	AAAA
ATOM	2750	NH1	ARG	344	15.805	50.668	56.835	1.00	29.63	AAAA
ATOM	2751	NH2	ARG	344	15.379	49.198	55.120	1.00	27.19	AAAA
ATOM	2752	C	ARG	344	20.116	55.769	55.660	1.00	34.31	AAAA
ATOM	2753	O	ARG	344	21.005	55.557	56.391	1.00	29.09	AAAA
ATOM	2754	N	SER	345	20.011	56.745	55.294	1.00	28.34	AAAA
ATOM	2755	CA	SER	345	20.999	57.839	55.715	1.00	30.95	AAAA
ATOM	2756	CB	SER	345	20.669	59.199	55.109	1.00	29.56	AAAA
ATOM	2757	OG	SER	345	19.429	59.648	55.610	1.00	29.38	AAAA
ATOM	2758	C	SER	345	21.137	57.988	57.230	1.00	30.92	AAAA
ATOM	2759	O	SER	345	22.155	58.488	57.718	1.00	31.15	AAAA
ATOM	2760	N	TYR	346	20.116	57.576	57.975	1.00	25.64	AAAA
ATOM	2761	CA	TYR	346	20.158	57.659	59.433	1.00	26.81	AAAA
ATOM	2762	CB	TYR	346	18.823	57.189	60.006	1.00	34.41	AAAA
ATOM	2763	CG	TYR	346	18.529	55.723	59.716	1.00	27.35	AAAA
ATOM	2764	CD1	TYR	346	19.003	54.708	60.556	1.00	24.87	AAAA
ATOM	2765	CE1	TYR	346	18.744	53.352	60.278	1.00	28.05	AAAA
ATOM	2766	CD2	TYR	346	17.795	55.358	58.588	1.00	27.70	AAAA
ATOM	2767	CE2	TYR	346	17.533	54.008	58.297	1.00	26.59	AAAA
ATOM	2768	CZ	TYR	346	18.008	53.015	59.145	1.00	33.75	AAAA
ATOM	2769	OH	TYR	346	17.737	51.691	58.855	1.00	26.06	AAAA
ATOM	2770	C	TYR	346	21.277	56.766	59.977	1.00	25.57	AAA
ATOM	2771	O	TYR	346	21.769	56.970	61.085	1.00	28.07	AAA
ATOM	2772	N	MET	347	21.666	55.761	59.198	1.00	29.08	AAA

61/263

Figure 16-43

ATOM	2773	CA	MET	347	22.720	54.837	59.622	1.00	24.19	AAAA
ATOM	2774	CB	MET	347	22.844	53.678	58.628	1.00	24.87	AAAA
ATOM	2775	CG	MET	347	21.609	52.806	58.543	1.00	23.66	AAAA
ATOM	2776	SD	MET	347	21.780	51.503	57.267	1.00	27.02	AAAA
ATOM	2777	CE	MET	347	22.115	52.375	55.896	1.00	37.69	AAAA
ATOM	2778	C	MET	347	24.054	55.540	59.737	1.00	29.45	AAAA
ATOM	2779	O	MET	347	24.937	55.092	60.479	1.00	28.08	AAAA
ATOM	2780	N	LEU	348	24.188	56.650	59.007	1.00	23.71	AAAA
ATOM	2781	CA	LEU	348	25.418	57.446	58.998	1.00	34.11	AAAA
ATOM	2782	CB	LEU	348	25.463	58.351	57.757	1.00	25.37	AAAA
ATOM	2783	CG	LEU	348	25.320	57.785	56.344	1.00	30.38	AAAA
ATOM	2784	CD1	LEU	348	25.307	58.944	55.340	1.00	27.44	AAAA
ATOM	2785	CD2	LEU	348	26.459	56.814	56.041	1.00	36.44	AAAA
ATOM	2786	C	LEU	348	25.507	58.332	60.237	1.00	36.09	AAAA
ATOM	2787	O	LEU	348	26.561	58.894	60.539	1.00	33.30	AAAA
ATOM	2788	N	GLU	349	24.394	58.445	60.953	1.00	30.51	AAAA
ATOM	2789	CA	GLU	349	24.313	59.292	62.136	1.00	35.53	AAAA
ATOM	2790	CB	GLU	349	22.908	59.896	62.217	1.00	31.35	AAAA
ATOM	2791	CG	GLU	349	22.518	60.717	61.006	1.00	29.09	AAAA
ATOM	2792	CD	GLU	349	23.481	61.859	60.746	1.00	31.78	AAAA
ATOM	2793	OE1	GLU	349	23.937	62.476	61.730	1.00	30.98	AAAA
ATOM	2794	OE2	GLU	349	23.766	62.155	59.569	1.00	30.67	AAAA
ATOM	2795	C	GLU	349	24.663	58.633	63.471	1.00	38.48	AAAA
ATOM	2796	O	GLU	349	24.727	59.303	64.502	1.00	40.12	AAAA
ATOM	2797	N	THR	350	24.878	57.326	63.461	1.00	33.58	AAAA
ATOM	2798	CA	THR	350	25.221	56.612	64.681	1.00	29.74	AAAA
ATOM	2799	CB	THR	350	23.992	56.363	65.559	1.00	35.91	AAAA
ATOM	2800	OG1	THR	350	23.421	57.615	65.952	1.00	45.03	AAAA
ATOM	2801	CG2	THR	350	24.382	55.586	66.806	1.00	49.48	AAAA
ATOM	2802	C	THR	350	25.821	55.267	64.330	1.00	30.63	AAAA
ATOM	2803	O	THR	350	25.535	54.709	63.274	1.00	26.62	AAAA
ATOM	2804	N	LEU	351	26.644	54.740	65.225	1.00	29.07	AAAA
ATOM	2805	CA	LEU	351	27.271	53.461	64.972	1.00	24.59	AAAA
ATOM	2806	CB	LEU	351	28.584	53.367	65.757	1.00	29.91	AAAA
ATOM	2807	CG	LEU	351	29.591	52.327	65.267	1.00	39.62	AAAA
ATOM	2808	CD1	LEU	351	30.887	52.467	66.039	1.00	37.09	AAAA
ATOM	2809	CD2	LEU	351	29.024	50.935	65.415	1.00	54.03	AAAA
ATOM	2810	C	LEU	351	26.314	52.336	65.377	1.00	29.71	AAAA
ATOM	2811	O	LEU	351	26.130	51.364	64.641	1.00	30.53	AAAA
ATOM	2812	N	LYS	352	25.697	52.481	66.543	1.00	28.64	AAAA
ATOM	2813	CA	LYS	352	24.763	51.479	67.061	1.00	32.72	AAAA
ATOM	2814	CB	LYS	352	24.913	51.381	68.581	1.00	27.37	AAAA
ATOM	2815	CG	LYS	352	26.230	50.787	69.034	1.00	43.48	AAAA
ATOM	2816	CD	LYS	352	26.536	51.068	70.504	1.00	46.77	AAAA
ATOM	2817	CE	LYS	352	25.484	50.538	71.451	1.00	51.52	AAAA
ATOM	2818	NZ	LYS	352	25.850	50.859	72.866	1.00	62.08	AAAA
ATOM	2819	C	LYS	352	23.330	51.856	66.731	1.00	32.49	AAAA
ATOM	2820	O	LYS	352	22.953	53.010	66.882	1.00	31.90	AAAA
ATOM	2821	N	ASP	353	22.525	50.916	66.244	1.00	31.44	AAAA
ATOM	2822	CA	ASP	353	21.136	51.286	66.012	1.00	26.50	AAAA
ATOM	2823	CB	ASP	353	20.543	50.635	64.746	1.00	50.09	AAAA
ATOM	2824	CG	ASP	353	20.880	49.176	64.604	1.00	52.79	AAAA
ATOM	2825	OD1	ASP	353	21.980	48.861	64.109	1.00	58.55	AAAA
ATOM	2826	OD2	ASP	353	20.040	48.339	64.984	1.00	73.19	AAAA
ATOM	2827	C	ASP	353	20.328	50.930	67.257	1.00	26.41	AAAA
ATOM	2828	O	ASP	353	20.806	50.214	68.136	1.00	25.73	AAAA
ATOM	2829	N	PRO	354	19.118	51.481	67.385	1.00	30.12	AAAA
ATOM	2830	CD	PRO	354	18.428	52.429	66.495	1.00	35.38	AAAA
ATOM	2831	CA	PRO	354	18.276	51.190	68.547	1.00	34.02	AAAA
ATOM	2832	CB	PRO	354	17.091	52.129	68.340	1.00	32.25	AAAA
ATOM	2833	CG	PRO	354	16.974	52.139	66.833	1.00	44.48	AAAA
ATOM	2834	C	PRO	354	17.838	49.736	68.512	1.00	34.00	AAAA
ATOM	2835	O	PRO	354	17.829	49.111	67.452	1.00	28.28	AAAA
ATOM	2836	N	TRP	355	17.484	49.190	69.664	1.00	23.89	AAAA
ATOM	2837	CA	TRP	355	17.010	47.818	69.669	1.00	33.84	AAAA
ATOM	2838	CB	TRP	355	16.653	47.363	71.076	1.00	33.84	AAAA

Figure 16-44

ATOM	2839	CG	TRP	355	17.844	46.946	71.832	1.00	49.97	AAAA
ATOM	2840	CD2	TRP	355	18.364	45.622	71.905	1.00	46.60	AAAA
ATOM	2841	CE2	TRP	355	19.567	45.682	72.639	1.00	54.73	AAAA
ATOM	2842	CE3	TRP	355	17.931	44.386	71.419	1.00	46.90	AAAA
ATOM	2843	CD1	TRP	355	18.723	47.746	72.507	1.00	56.10	AAAA
ATOM	2844	NE1	TRP	355	19.765	46.991	72.997	1.00	56.07	AAAA
ATOM	2845	CZ2	TRP	355	20.340	44.552	72.897	1.00	55.25	AAAA
ATOM	2846	CZ3	TRP	355	18.696	43.267	71.674	1.00	50.74	AAAA
ATOM	2847	CH2	TRP	355	19.887	43.356	72.405	1.00	50.68	AAAA
ATOM	2848	C	TRP	355	15.789	47.712	68.776	1.00	33.12	AAAA
ATOM	2849	O	TRP	355	15.096	48.705	68.550	1.00	29.41	AAAA
ATOM	2850	N	ARG	356	15.547	46.508	68.263	1.00	23.90	AAAA
ATOM	2851	CA	ARG	356	14.413	46.237	67.387	1.00	23.96	AAAA
ATOM	2852	CB	ARG	356	14.892	46.096	65.935	1.00	22.66	AAAA
ATOM	2853	CG	ARG	356	15.505	47.385	65.393	1.00	29.06	AAAA
ATOM	2854	CD	ARG	356	16.291	47.212	64.108	1.00	28.92	AAAA
ATOM	2855	NE	ARG	356	16.833	48.503	63.686	1.00	24.73	AAAA
ATOM	2856	CZ	ARG	356	17.733	48.668	62.724	1.00	23.57	AAAA
ATOM	2857	NH1	ARG	356	18.209	47.616	62.066	1.00	22.15	AAAA
ATOM	2858	NH2	ARG	356	18.153	49.891	62.418	1.00	22.69	AAAA
ATOM	2859	C	ARG	356	13.781	44.944	57.878	1.00	24.89	AAAA
ATOM	2860	O	ARG	356	13.785	43.925	57.189	1.00	22.25	AAAA
ATOM	2861	N	GLY	357	13.231	44.993	69.085	1.00	23.91	AAAA
ATOM	2862	CA	GLY	357	12.631	43.805	69.657	1.00	26.72	AAAA
ATOM	2863	C	GLY	357	11.138	43.671	69.465	1.00	26.90	AAAA
ATOM	2864	O	GLY	357	10.536	44.330	68.619	1.00	29.87	AAAA
ATOM	2865	N	GLY	358	10.544	42.797	70.265	1.00	28.22	AAAA
ATOM	2866	CA	GLY	358	9.118	42.561	70.188	1.00	30.96	AAAA
ATOM	2867	C	GLY	358	8.800	41.274	70.920	1.00	30.03	AAAA
ATOM	2868	O	GLY	358	9.626	40.757	71.663	1.00	24.03	AAAA
ATOM	2869	N	GLU	359	7.601	40.747	70.715	1.00	28.34	AAAA
ATOM	2870	CA	GLU	359	7.218	39.509	71.366	1.00	24.37	AAAA
ATOM	2871	CB	GLU	359	5.699	39.372	71.375	1.00	32.52	AAAA
ATOM	2872	CG	GLU	359	4.981	40.327	72.299	1.00	45.44	AAAA
ATOM	2873	CD	GLU	359	3.472	40.250	72.132	1.00	50.43	AAAA
ATOM	2874	OE1	GLU	359	2.924	39.125	72.151	1.00	42.92	AAAA
ATOM	2875	OE2	GLU	359	2.839	41.316	71.987	1.00	40.72	AAAA
ATOM	2876	C	GLU	359	7.804	38.323	70.628	1.00	27.35	AAAA
ATOM	2877	O	GLU	359	8.138	38.415	69.449	1.00	22.94	AAAA
ATOM	2878	N	VAL	360	7.944	37.208	71.325	1.00	19.68	AAAA
ATOM	2879	CA	VAL	360	8.441	36.017	70.672	1.00	21.28	AAAA
ATOM	2880	CB	VAL	360	9.300	35.188	71.621	1.00	26.71	AAAA
ATOM	2881	CG1	VAL	360	9.783	33.917	70.912	1.00	20.64	AAAA
ATOM	2882	CG2	VAL	360	10.486	36.038	72.113	1.00	25.79	AAAA
ATOM	2883	C	VAL	360	7.228	35.202	70.197	1.00	25.51	AAAA
ATOM	2884	O	VAL	360	6.442	34.700	71.011	1.00	19.75	AAAA
ATOM	2885	N	ARG	361	7.065	35.094	68.873	1.00	18.48	AAAA
ATOM	2886	CA	ARG	361	5.947	34.337	68.301	1.00	22.01	AAAA
ATOM	2887	CB	ARG	361	5.988	34.389	66.772	1.00	19.31	AAAA
ATOM	2888	CG	ARG	361	5.446	35.671	66.204	1.00	30.86	AAAA
ATOM	2889	CD	ARG	361	5.735	35.730	64.723	1.00	37.95	AAAA
ATOM	2890	NE	ARG	361	7.111	36.148	64.460	1.00	30.73	AAAA
ATOM	2891	CZ	ARG	361	7.616	36.275	63.242	1.00	22.89	AAAA
ATOM	2892	NH1	ARG	361	6.851	36.006	62.186	1.00	19.02	AAAA
ATOM	2893	NH2	ARG	361	8.861	36.704	63.081	1.00	23.47	AAAA
ATOM	2894	C	ARG	361	5.897	32.879	68.714	1.00	26.11	AAAA
ATOM	2895	O	ARG	361	6.926	32.255	68.968	1.00	21.79	AAAA
ATOM	2896	N	LYS	362	4.681	32.338	68.763	1.00	24.89	AAAA
ATOM	2897	CA	LYS	362	4.479	30.938	69.125	1.00	28.63	AAAA
ATOM	2898	CB	LYS	362	2.981	30.570	69.070	1.00	22.91	AAAA
ATOM	2899	CG	LYS	362	2.145	31.200	70.168	1.00	50.86	AAAA
ATOM	2900	CD	LYS	362	2.290	32.715	70.157	1.00	57.51	AAAA
ATOM	2901	CE	LYS	362	1.923	33.278	68.799	1.00	50.87	AAAA
ATOM	2902	NZ	LYS	362	2.307	34.683	68.711	1.00	22.99	AAAA
ATOM	2903	C	LYS	362	5.269	30.014	68.202	1.00	16.77	AAAA
ATOM	2904	O	LYS	362	5.808	29.007	68.647	1.00	22.90	AAAA

Figure 16-45

ATOM	2905	N	GLU	363	5.311	30.355	66.913	1.00	25.24	AAAA
ATOM	2906	CA	GLU	363	6.055	29.577	65.910	1.00	26.29	AAAA
ATOM	2907	CB	GLU	363	6.207	30.342	64.608	1.00	33.50	AAAA
ATOM	2908	CG	GLU	363	4.999	30.639	63.824	1.00	48.73	AAAA
ATOM	2909	CD	GLU	363	5.368	31.494	62.638	1.00	42.01	AAAA
ATOM	2910	OE1	GLU	363	6.299	31.087	61.895	1.00	28.50	AAAA
ATOM	2911	OE2	GLU	363	4.738	32.558	62.461	1.00	44.91	AAAA
ATOM	2912	C	GLU	363	7.481	29.326	66.349	1.00	19.00	AAAA
ATOM	2913	O	GLU	363	8.011	28.218	66.226	1.00	18.66	AAAA
ATOM	2914	N	VAL	364	8.121	30.399	66.790	1.00	20.69	AAAA
ATOM	2915	CA	VAL	364	9.501	30.303	67.219	1.00	23.13	AAAA
ATOM	2916	CB	VAL	364	10.096	31.681	67.510	1.00	16.98	AAAA
ATOM	2917	CG1	VAL	364	11.515	31.513	68.010	1.00	22.32	AAAA
ATOM	2918	CG2	VAL	364	10.082	32.548	66.242	1.00	23.99	AAAA
ATOM	2919	C	VAL	364	9.625	29.415	68.448	1.00	19.28	AAAA
ATOM	2920	O	VAL	364	10.507	28.548	68.510	1.00	20.17	AAAA
ATOM	2921	N	LYS	365	8.735	29.600	69.417	1.00	21.11	AAAA
ATOM	2922	CA	LYS	365	8.780	28.768	70.612	1.00	18.15	AAAA
ATOM	2923	CB	LYS	365	7.711	29.210	71.626	1.00	25.22	AAAA
ATOM	2924	CG	LYS	365	7.921	30.611	72.167	1.00	32.99	AAAA
ATOM	2925	CD	LYS	365	6.901	30.949	73.253	1.00	36.09	AAAA
ATOM	2926	CE	LYS	365	7.121	32.357	73.790	1.00	28.99	AAAA
ATOM	2927	NZ	LYS	365	6.178	32.736	74.882	1.00	38.98	AAAA
ATOM	2928	C	LYS	365	8.574	27.305	70.236	1.00	19.49	AAAA
ATOM	2929	O	LYS	365	9.255	26.417	70.758	1.00	22.04	AAAA
ATOM	2930	N	ASP	366	7.635	27.048	69.327	1.00	22.45	AAAA
ATOM	2931	CA	ASP	366	7.386	25.669	68.915	1.00	22.62	AAAA
ATOM	2932	CB	ASP	366	6.173	25.574	67.967	1.00	21.69	AAAA
ATOM	2933	CG	ASP	366	4.870	25.987	68.634	1.00	27.75	AAAA
ATOM	2934	OD1	ASP	366	4.763	25.890	69.881	1.00	31.01	AAAA
ATOM	2935	OD2	ASP	366	3.938	26.382	67.907	1.00	33.20	AAAA
ATOM	2936	C	ASP	366	8.606	25.034	68.237	1.00	24.53	AAAA
ATOM	2937	O	ASP	366	8.924	23.871	68.480	1.00	21.13	AAAA
ATOM	2938	N	THR	367	9.281	25.787	67.380	1.00	26.19	AAAA
ATOM	2939	CA	THR	367	10.462	25.252	66.694	1.00	21.68	AAAA
ATOM	2940	CB	THR	367	11.035	26.301	65.742	1.00	14.56	AAAA
ATOM	2941	CG1	THR	367	10.085	26.545	64.697	1.00	21.76	AAAA
ATOM	2942	CG2	THR	367	12.340	25.825	65.138	1.00	19.83	AAAA
ATOM	2943	C	THR	367	11.523	24.822	67.710	1.00	19.02	AAAA
ATOM	2944	O	THR	367	12.071	23.717	67.625	1.00	21.79	AAAA
ATOM	2945	N	LEU	368	11.802	25.684	68.683	1.00	18.42	AAAA
ATOM	2946	CA	LEU	368	12.797	25.348	69.700	1.00	21.02	AAAA
ATOM	2947	CB	LEU	368	13.148	26.569	70.560	1.00	17.34	AAAA
ATOM	2948	CG	LEU	368	14.206	27.518	69.959	1.00	17.45	AAAA
ATOM	2949	CD1	LEU	368	15.525	26.758	69.817	1.00	16.83	AAAA
ATOM	2950	CD2	LEU	368	13.756	28.041	68.593	1.00	19.49	AAAA
ATOM	2951	C	LEU	368	12.361	24.189	70.589	1.00	23.17	AAAA
ATOM	2952	O	LEU	368	13.203	23.420	71.052	1.00	24.81	AAAA
ATOM	2953	N	GLU	369	11.059	24.055	70.839	1.00	23.97	AAAA
ATOM	2954	CA	GLU	369	10.597	22.929	71.653	1.00	19.36	AAAA
ATOM	2955	CB	GLU	369	9.127	23.113	72.063	1.00	21.81	AAAA
ATOM	2956	CG	GLU	369	8.913	24.225	73.100	1.00	40.15	AAAA
ATOM	2957	CD	GLU	369	7.450	24.416	73.487	1.00	49.38	AAAA
ATOM	2958	OE1	GLU	369	6.806	23.429	73.905	1.00	43.26	AAAA
ATOM	2959	OE2	GLU	369	6.948	25.558	73.382	1.00	57.31	AAAA
ATOM	2960	C	GLU	369	10.778	21.623	70.859	1.00	24.29	AAAA
ATOM	2961	O	GLU	369	11.172	20.605	71.420	1.00	25.96	AAAA
ATOM	2962	N	LYS	370	10.488	21.643	69.560	1.00	22.98	AAAA
ATOM	2963	CA	LYS	370	10.665	20.437	68.746	1.00	23.19	AAAA
ATOM	2964	CB	LYS	370	10.051	20.596	67.347	1.00	26.83	AAAA
ATOM	2965	CG	LYS	370	8.537	20.461	67.287	1.00	36.68	AAAA
ATOM	2966	CD	LYS	370	8.056	20.431	65.832	1.00	39.85	AAAA
ATOM	2967	CE	LYS	370	6.567	20.105	65.740	1.00	56.23	AAAA
ATOM	2968	NZ	LYS	370	6.082	19.996	64.326	1.00	56.10	AAAA
ATOM	2969	C	LYS	370	12.148	20.123	68.602	1.00	31.63	AAAA
ATOM	2970	O	LYS	370	12.549	18.958	68.587	1.00	36.88	AAAA

ATOM	2971	N	ALA	371	12.961	21.170	68.491	1.00	26.25	AAAA
ATOM	2972	CA	ALA	371	14.407	21.009	68.360	1.00	27.33	AAAA
ATOM	2973	CB	ALA	371	15.079	22.370	68.188	1.00	23.70	AAAA
ATOM	2974	C	ALA	371	14.989	20.308	69.581	1.00	26.74	AAAA
ATOM	2975	O	ALA	371	15.892	19.482	69.452	1.00	29.52	AAAA
ATOM	2976	N	ALA	372	14.484	20.652	70.764	1.00	24.83	AAAA
ATOM	2977	CA	ALA	372	14.959	20.055	72.012	1.00	34.24	AAAA
ATOM	2978	CB	ALA	372	14.305	20.750	73.214	1.00	37.17	AAAA
ATOM	2979	C	ALA	372	14.663	18.564	72.061	1.00	45.62	AAAA
ATOM	2980	O	ALA	372	15.563	17.741	72.280	1.00	35.52	AAAA
ATOM	2981	N	ALA	373	13.394	18.216	71.869	1.00	44.50	AAAA
ATOM	2982	CA	ALA	373	13.004	16.813	71.892	1.00	49.88	AAAA
ATOM	2983	CB	ALA	373	11.506	16.681	71.628	1.00	49.32	AAAA
ATOM	2984	C	ALA	373	13.807	16.072	70.825	1.00	44.64	AAAA
ATOM	2985	O	ALA	373	14.669	15.250	71.201	1.00	58.19	AAAA
ATOM	2986	OXT	ALA	373	13.591	16.337	69.626	1.00	41.63	AAAA
HETATM	2987	OH2	WAT	1	36.368	43.907	49.242	1.00	13.03	SOLV
HETATM	2988	OH2	WAT	2	23.107	30.584	59.802	1.00	11.42	SOLV
HETATM	2989	OH2	WAT	3	20.594	33.744	61.457	1.00	14.73	SOLV
HETATM	2990	OH2	WAT	4	31.359	16.551	51.590	1.00	19.84	SOLV
HETATM	2991	OH2	WAT	5	30.389	18.140	45.769	1.00	19.94	SOLV
HETATM	2992	OH2	WAT	6	16.925	41.748	56.551	1.00	13.33	SOLV
HETATM	2993	OH2	WAT	7	28.448	16.084	62.316	1.00	14.08	SOLV
HETATM	2994	OH2	WAT	8	40.375	38.476	55.678	1.00	19.10	SOLV
HETATM	2995	OH2	WAT	9	18.455	29.667	54.797	1.00	18.81	SOLV
HETATM	2996	OH2	WAT	10	26.305	18.390	59.507	1.00	16.65	SOLV
HETATM	2997	OH2	WAT	11	50.145	32.063	58.142	1.00	16.53	SOLV
HETATM	2998	OH2	WAT	12	45.935	30.996	40.672	1.00	25.08	SOLV
HETATM	2999	OH2	WAT	13	26.358	43.110	74.179	1.00	22.91	SOLV
HETATM	3000	OH2	WAT	14	48.727	24.720	56.917	1.00	25.49	SOLV
HETATM	3001	OH2	WAT	15	30.244	18.663	50.165	1.00	25.78	SOLV
HETATM	3002	OH2	WAT	16	10.615	28.799	63.631	1.00	22.40	SOLV
HETATM	3003	OH2	WAT	17	18.401	20.018	62.704	1.00	21.46	SOLV
HETATM	3004	OH2	WAT	18	22.195	47.791	60.896	1.00	26.19	SOLV
HETATM	3005	OH2	WAT	19	3.278	32.141	65.350	1.00	20.38	SOLV
HETATM	3006	OH2	WAT	20	23.643	22.897	59.512	1.00	21.27	SOLV
HETATM	3007	OH2	WAT	21	50.287	23.101	48.818	1.00	19.73	SOLV
HETATM	3008	OH2	WAT	22	44.725	34.256	46.541	1.00	18.74	SOLV
HETATM	3009	OH2	WAT	23	8.346	30.527	49.922	1.00	22.33	SOLV
HETATM	3010	OH2	WAT	24	39.855	33.795	67.390	1.00	20.43	SOLV
HETATM	3011	OH2	WAT	25	7.827	32.763	57.779	1.00	19.24	SOLV
HETATM	3012	OH2	WAT	26	45.388	34.567	36.246	1.00	20.86	SOLV
HETATM	3013	OH2	WAT	27	47.636	32.244	33.388	1.00	20.41	SOLV
HETATM	3014	OH2	WAT	28	32.514	35.684	41.278	1.00	24.76	SOLV
HETATM	3015	OH2	WAT	29	26.188	15.341	61.913	1.00	19.63	SOLV
HETATM	3016	OH2	WAT	30	14.957	43.169	56.333	1.00	23.80	SOLV
HETATM	3017	OH2	WAT	31	24.483	43.556	55.704	1.00	27.25	SOLV
HETATM	3018	OH2	WAT	32	41.141	16.376	48.456	1.00	25.99	SOLV
HETATM	3019	OH2	WAT	33	23.104	17.625	54.086	1.00	26.37	SOLV
HETATM	3020	OH2	WAT	34	51.301	28.602	57.694	1.00	32.78	SOLV
HETATM	3021	OH2	WAT	35	51.376	29.469	53.156	1.00	24.27	SOLV
HETATM	3022	OH2	WAT	36	12.518	22.131	49.816	1.00	23.60	SOLV
HETATM	3023	OH2	WAT	37	6.521	27.442	50.861	1.00	25.87	SOLV
HETATM	3024	OH2	WAT	38	30.390	33.757	34.190	1.00	19.87	SOLV
HETATM	3025	OH2	WAT	39	8.328	29.586	62.062	1.00	32.01	SOLV
HETATM	3026	OH2	WAT	40	30.180	24.235	30.724	1.00	22.61	SOLV
HETATM	3027	OH2	WAT	41	44.521	30.663	38.395	1.00	27.52	SOLV
HETATM	3028	OH2	WAT	42	30.981	18.043	41.186	1.00	23.45	SOLV
HETATM	3029	OH2	WAT	43	14.632	37.127	73.830	1.00	29.36	SOLV
HETATM	3030	OH2	WAT	44	39.332	25.953	72.230	1.00	21.87	SOLV
HETATM	3031	OH2	WAT	45	7.597	37.592	51.896	1.00	39.62	SOLV
HETATM	3032	OH2	WAT	46	15.027	18.079	54.827	1.00	26.65	SOLV
HETATM	3033	OH2	WAT	47	11.076	45.493	66.435	1.00	38.18	SOLV
HETATM	3034	OH2	WAT	48	42.124	18.055	37.233	1.00	28.62	SOLV
HETATM	3035	OH2	WAT	49	48.736	25.764	64.149	1.00	31.88	SOLV
HETATM	3036	OH2	WAT	50	50.383	27.254	54.972	1.00	24.36	SOLV

65/263 Figure 16-47

HETATM	3037	OH2	WAT	51	48.659	36.025	68.226	1.00	33.89	SOLV
HETATM	3038	OH2	WAT	52	36.998	27.228	71.440	1.00	21.03	SOLV
HETATM	3039	OH2	WAT	53	41.303	16.309	55.307	1.00	32.23	SOLV
HETATM	3040	OH2	WAT	54	33.242	39.524	49.454	1.00	29.77	SOLV
HETATM	3041	OH2	WAT	55	45.004	25.973	35.031	1.00	21.59	SOLV
HETATM	3042	OH2	WAT	56	19.039	25.829	45.793	1.00	33.48	SOLV
HETATM	3043	OH2	WAT	57	17.922	35.542	50.154	1.00	37.51	SOLV
HETATM	3044	OH2	WAT	58	10.409	26.864	73.166	1.00	26.54	SOLV
HETATM	3045	OH2	WAT	59	11.835	22.805	59.408	1.00	20.83	SOLV
HETATM	3046	OH2	WAT	60	18.254	48.699	53.224	1.00	28.41	SOLV
HETATM	3047	OH2	WAT	61	10.426	26.647	60.447	1.00	32.72	SOLV
HETATM	3048	OH2	WAT	62	21.304	55.086	63.510	1.00	28.84	SOLV
HETATM	3049	OH2	WAT	63	32.532	51.211	45.469	1.00	32.48	SOLV
HETATM	3050	OH2	WAT	64	22.658	61.079	57.420	1.00	27.32	SOLV
HETATM	3051	OH2	WAT	65	16.734	24.334	74.721	1.00	27.44	SOLV
HETATM	3052	OH2	WAT	66	32.758	37.824	54.391	1.00	25.07	SOLV
HETATM	3053	OH2	WAT	67	11.142	25.859	49.706	1.00	29.66	SOLV
HETATM	3054	OH2	WAT	68	24.192	15.261	53.236	1.00	30.21	SOLV
HETATM	3055	OH2	WAT	69	19.816	17.916	66.357	1.00	30.50	SOLV
HETATM	3056	OH2	WAT	70	50.347	23.975	53.197	1.00	28.08	SOLV
HETATM	3057	OH2	WAT	71	50.258	30.918	51.113	1.00	20.19	SOLV
HETATM	3058	OH2	WAT	72	21.047	17.624	68.693	1.00	41.23	SOLV
HETATM	3059	OH2	WAT	73	26.782	33.756	49.995	1.00	25.80	SOLV
HETATM	3060	OH2	WAT	74	12.570	43.844	64.441	1.00	31.03	SOLV
HETATM	3061	OH2	WAT	75	35.555	41.287	50.852	1.00	24.03	SOLV
HETATM	3062	OH2	WAT	76	27.764	18.231	61.827	1.00	18.28	SOLV
HETATM	3063	OH2	WAT	77	26.715	29.236	38.391	1.00	23.18	SOLV
HETATM	3064	OH2	WAT	78	21.461	23.245	48.872	1.00	23.80	SOLV
HETATM	3065	OH2	WAT	79	49.246	28.263	65.477	1.00	21.52	SOLV
HETATM	3066	OH2	WAT	80	31.785	13.301	69.606	1.00	31.11	SOLV
HETATM	3067	OH2	WAT	81	49.811	34.740	59.229	1.00	31.76	SOLV
HETATM	3068	OH2	WAT	82	45.670	33.188	42.470	1.00	23.13	SOLV
HETATM	3069	OH2	WAT	83	9.408	39.751	55.872	1.00	31.53	SOLV
HETATM	3070	OH2	WAT	84	35.166	35.878	29.899	1.00	37.32	SOLV
HETATM	3071	OH2	WAT	85	41.927	22.970	73.694	1.00	44.07	SOLV
HETATM	3072	OH2	WAT	86	22.125	34.577	49.199	1.00	44.65	SOLV
HETATM	3073	OH2	WAT	87	43.984	33.541	37.965	1.00	24.88	SOLV
HETATM	3074	OH2	WAT	88	11.997	17.962	56.312	1.00	34.85	SOLV
HETATM	3075	OH2	WAT	89	42.194	14.737	59.766	1.00	25.91	SOLV
HETATM	3076	OH2	WAT	90	49.313	24.200	41.684	1.00	29.29	SOLV
HETATM	3077	OH2	WAT	91	48.504	33.595	61.519	1.00	30.32	SOLV
HETATM	3078	OH2	WAT	92	24.773	18.356	33.365	1.00	53.13	SOLV
HETATM	3079	OH2	WAT	93	35.160	35.656	47.470	1.00	41.41	SOLV
HETATM	3080	OH2	WAT	94	44.682	36.658	39.962	1.00	29.24	SOLV
HETATM	3081	OH2	WAT	95	9.576	41.033	52.549	1.00	51.83	SOLV
HETATM	3082	OH2	WAT	96	47.199	20.112	42.102	1.00	40.39	SOLV
HETATM	3083	OH2	WAT	97	49.254	26.331	59.641	1.00	37.03	SOLV
HETATM	3084	OH2	WAT	98	26.808	37.600	38.172	1.00	28.74	SOLV
HETATM	3085	OH2	WAT	99	40.749	14.572	64.635	1.00	33.42	SOLV
HETATM	3086	OH2	WAT	100	24.850	44.161	47.775	1.00	27.89	SOLV
HETATM	3087	OH2	WAT	101	34.326	42.063	46.714	1.00	42.22	SOLV
HETATM	3088	OH2	WAT	102	30.226	34.544	52.026	1.00	30.77	SOLV
HETATM	3089	OH2	WAT	103	47.824	39.054	78.097	1.00	52.16	SOLV
HETATM	3090	OH2	WAT	104	19.665	18.953	47.438	1.00	51.70	SOLV
HETATM	3091	OH2	WAT	105	46.857	36.525	46.232	1.00	23.65	SOLV
HETATM	3092	OH2	WAT	106	48.069	19.460	67.360	1.00	37.56	SOLV
HETATM	3093	OH2	WAT	107	15.553	56.850	61.838	1.00	46.95	SOLV
HETATM	3094	OH2	WAT	108	44.026	19.119	70.671	1.00	39.55	SOLV
HETATM	3095	OH2	WAT	109	8.139	42.064	65.674	1.00	42.61	SOLV
HETATM	3096	OH2	WAT	110	50.624	36.591	65.779	1.00	31.59	SOLV
HETATM	3097	OH2	WAT	111	51.398	26.073	61.043	1.00	49.09	SOLV
HETATM	3098	OH2	WAT	112	26.174	33.692	33.551	1.00	36.61	SOLV
HETATM	3099	OH2	WAT	113	23.545	20.203	53.001	1.00	24.34	SOLV
HETATM	3100	OH2	WAT	114	9.083	42.965	57.697	1.00	33.65	SOLV
HETATM	3101	OH2	WAT	115	8.442	39.898	64.594	1.00	31.21	SOLV
HETATM	3102	OH2	WAT	116	15.219	35.897	51.951	1.00	26.59	SOLV

HETATM	3103	OH2	WAT	117	15.417	38.438	50.473	1.00	34.46	SOLV
HETATM	3104	OH2	WAT	118	40.757	26.310	29.206	1.00	29.12	SOLV
HETATM	3105	OH2	WAT	119	27.717	18.542	46.553	1.00	28.17	SOLV
HETATM	3106	OH2	WAT	120	18.612	13.786	56.845	1.00	38.56	SOLV
HETATM	3107	OH2	WAT	121	43.198	31.377	72.139	1.00	26.31	SOLV
HETATM	3108	OH2	WAT	122	44.188	35.704	33.802	1.00	29.81	SOLV
HETATM	3109	OH2	WAT	123	50.736	40.909	58.456	1.00	32.40	SOLV
HETATM	3110	OH2	WAT	124	31.302	33.760	31.742	1.00	30.84	SOLV
HETATM	3111	OH2	WAT	125	36.895	21.264	34.198	1.00	34.67	SOLV
HETATM	3112	OH2	WAT	126	47.474	22.252	67.427	1.00	34.35	SOLV
HETATM	3113	OH2	WAT	127	7.178	25.936	64.063	1.00	31.77	SOLV
HETATM	3114	OH2	WAT	128	36.362	66.647	54.021	1.00	36.88	SOLV
HETATM	3115	OH2	WAT	129	42.486	35.503	30.348	1.00	26.61	SOLV
HETATM	3116	OH2	WAT	130	8.432	34.383	50.442	1.00	37.45	SOLV
HETATM	3117	OH2	WAT	131	37.644	49.018	48.946	1.00	37.33	SOLV
HETATM	3118	OH2	WAT	132	50.273	41.645	63.380	1.00	37.33	SOLV
HETATM	3119	OH2	WAT	133	7.518	26.633	61.571	1.00	45.42	SOLV
HETATM	3120	OH2	WAT	134	31.483	46.197	72.538	1.00	28.02	SOLV
HETATM	3121	OH2	WAT	135	41.501	16.604	58.054	1.00	32.78	SOLV
HETATM	3122	OH2	WAT	136	45.898	47.740	55.185	1.00	43.47	SOLV
HETATM	3123	OH2	WAT	137	16.300	33.614	49.519	1.00	30.37	SOLV
HETATM	3124	OH2	WAT	138	51.148	36.946	55.148	1.00	46.34	SOLV
HETATM	3125	OH2	WAT	139	21.525	53.761	50.892	1.00	38.27	SOLV
HETATM	3126	OH2	WAT	140	21.603	54.580	68.690	1.00	33.10	SOLV
HETATM	3127	OH2	WAT	141	10.191	29.237	60.325	1.00	30.24	SOLV
HETATM	3128	OH2	WAT	142	16.951	18.120	66.901	1.00	40.85	SOLV
HETATM	3129	OH2	WAT	143	4.943	24.912	51.199	1.00	49.13	SOLV
HETATM	3130	OH2	WAT	144	10.711	25.291	58.177	1.00	30.72	SOLV
HETATM	3131	OH2	WAT	145	30.815	43.398	36.040	1.00	42.23	SOLV
HETATM	3132	OH2	WAT	146	21.763	24.512	46.695	1.00	28.31	SOLV
HETATM	3133	OH2	WAT	147	51.788	33.122	50.887	1.00	26.15	SOLV
HETATM	3134	OH2	WAT	148	24.531	44.741	72.420	1.00	27.99	SOLV
HETATM	3135	OH2	WAT	149	50.938	23.483	60.422	1.00	38.20	SOLV
HETATM	3136	OH2	WAT	150	24.860	47.932	61.067	1.00	18.89	SOLV
HETATM	3137	OH2	WAT	151	27.336	37.304	35.642	1.00	33.58	SOLV
HETATM	3138	OH2	WAT	152	38.680	35.535	35.974	1.00	26.89	SOLV
HETATM	3139	OH2	WAT	153	24.441	16.097	33.317	1.00	48.33	SOLV
HETATM	3140	OH2	WAT	154	20.343	18.124	73.416	1.00	36.28	SOLV
HETATM	3141	OH2	WAT	155	49.765	37.948	74.801	1.00	48.41	SOLV
HETATM	3142	OH2	WAT	156	34.329	31.169	47.547	1.00	25.33	SOLV
HETATM	3143	OH2	WAT	157	43.028	24.554	72.536	1.00	41.54	SOLV
HETATM	3144	OH2	WAT	158	39.888	15.082	42.035	1.00	28.76	SOLV
HETATM	3145	OH2	WAT	159	41.886	20.780	73.179	1.00	51.03	SOLV
HETATM	3146	OH2	WAT	160	22.962	49.969	58.518	1.00	35.04	SOLV
HETATM	3147	OH2	WAT	161	14.696	15.261	68.016	1.00	55.47	SOLV
HETATM	3148	OH2	WAT	162	14.915	18.181	64.866	1.00	42.00	SOLV
HETATM	3149	OH2	WAT	163	30.608	49.029	52.612	1.00	47.32	SOLV
HETATM	3150	OH2	WAT	164	52.566	30.906	57.612	1.00	36.71	SOLV
HETATM	3151	OH2	WAT	165	23.699	27.331	77.729	1.00	32.22	SOLV
HETATM	3152	OH2	WAT	166	36.971	59.046	63.272	1.00	43.05	SOLV
HETATM	3153	OH2	WAT	167	46.053	45.927	52.876	1.00	33.66	SOLV
HETATM	3154	OH2	WAT	168	42.780	49.151	58.106	1.00	44.63	SOLV
HETATM	3155	OH2	WAT	169	15.100	44.506	72.183	1.00	45.43	SOLV
HETATM	3156	OH2	WAT	170	31.677	60.998	50.050	1.00	34.51	SOLV
HETATM	3157	OH2	WAT	171	25.336	45.674	45.578	1.00	55.85	SOLV
HETATM	3158	OH2	WAT	172	17.481	18.266	49.018	1.00	32.73	SOLV
HETATM	3159	OH2	WAT	173	26.112	18.147	31.404	1.00	49.94	SOLV
HETATM	3160	OH2	WAT	174	45.874	43.142	70.985	1.00	32.89	SOLV
HETATM	3161	OH2	WAT	175	34.517	17.884	33.278	1.00	42.20	SOLV
HETATM	3162	OH2	WAT	176	16.330	54.886	50.466	1.00	40.74	SOLV
HETATM	3163	OH2	WAT	177	31.400	51.087	74.689	1.00	38.56	SOLV
HETATM	3164	OH2	WAT	178	50.971	27.079	67.130	1.00	44.49	SOLV
HETATM	3165	OH2	WAT	179	7.933	23.412	54.691	1.00	42.84	SOLV
HETATM	3166	OH2	WAT	180	33.498	47.596	73.612	1.00	35.99	SOLV
HETATM	3167	OH2	WAT	181	26.016	19.583	44.954	1.00	51.31	SOLV
HETATM	3168	OH2	WAT	182	40.139	17.026	74.920	1.00	43.64	SOLV

67/263

Figure 16-49

HETATM 3169	OH2 WAT	183	10.441	42.659	62.744	1.00	34.51	SOLV
HETATM 3170	OH2 WAT	184	2.095	34.482	65.810	1.00	36.49	SOLV
HETATM 3171	OH2 WAT	185	45.749	18.286	51.615	1.00	28.19	SOLV
HETATM 3172	OH2 WAT	186	25.771	38.332	76.707	1.00	45.53	SOLV
HETATM 3173	OH2 WAT	187	7.228	40.382	57.542	1.00	48.91	SOLV
HETATM 3174	OH2 WAT	188	42.972	52.824	67.739	1.00	39.99	SOLV
HETATM 3175	OH2 WAT	189	20.137	13.189	73.277	1.00	44.91	SOLV
HETATM 3176	OH2 WAT	190	48.945	19.193	47.581	1.00	52.88	SOLV
HETATM 3177	OH2 WAT	191	14.549	34.547	47.665	1.00	49.15	SOLV
HETATM 3178	OH2 WAT	192	31.765	20.567	26.536	1.00	42.23	SOLV
HETATM 3179	OH2 WAT	193	9.784	39.303	74.222	1.00	32.10	SOLV
HETATM 3180	OH2 WAT	194	28.865	12.481	52.375	1.00	50.98	SOLV
HETATM 3181	OH2 WAT	195	24.030	12.804	70.409	1.00	52.43	SOLV
HETATM 3182	OH2 WAT	196	47.209	39.536	50.698	1.00	43.03	SOLV
HETATM 3183	OH2 WAT	197	35.618	18.114	27.306	1.00	41.11	SOLV
HETATM 3184	OH2 WAT	198	23.625	48.145	43.853	1.00	48.20	SOLV
HETATM 3185	OH2 WAT	199	37.090	59.044	54.185	1.00	34.99	SOLV
HETATM 3186	OH2 WAT	200	34.478	12.208	59.080	1.00	36.58	SOLV
HETATM 3187	OH2 WAT	201	22.142	29.583	76.228	1.00	33.95	SOLV
HETATM 3188	OH2 WAT	202	13.608	42.619	53.973	1.00	40.44	SOLV
HETATM 3189	OH2 WAT	203	42.647	18.701	72.526	1.00	55.64	SOLV
HETATM 3190	OH2 WAT	204	37.005	35.993	77.480	1.00	34.82	SOLV
HETATM 3191	OH2 WAT	205	34.154	20.512	33.327	1.00	31.00	SOLV
HETATM 3192	OH2 WAT	206	37.264	57.546	47.642	1.00	49.58	SOLV
HETATM 3193	OH2 WAT	207	17.924	35.195	79.003	1.00	38.45	SOLV
HETATM 3194	OH2 WAT	208	51.172	31.581	62.378	1.00	35.37	SOLV
HETATM 3195	OH2 WAT	209	50.503	36.726	79.224	1.00	39.95	SOLV
HETATM 3196	OH2 WAT	210	18.382	13.162	63.852	1.00	52.08	SOLV
HETATM 3197	OH2 WAT	211	27.245	8.351	55.199	1.00	39.12	SOLV
HETATM 3198	OH2 WAT	212	18.354	13.545	59.540	1.00	30.15	SOLV
HETATM 3199	OH2 WAT	213	49.088	51.744	63.388	1.00	36.69	SOLV
HETATM 3200	OH2 WAT	214	23.251	33.160	50.871	1.00	42.11	SOLV
HETATM 3201	OH2 WAT	215	12.989	35.073	50.651	1.00	38.63	SOLV
HETATM 3202	OH2 WAT	216	24.414	44.460	43.239	1.00	37.93	SOLV
HETATM 3203	OH2 WAT	217	24.690	47.590	73.117	1.00	34.17	SOLV
HETATM 3204	OH2 WAT	218	19.844	17.949	81.360	1.00	40.74	SOLV
HETATM 3205	OH2 WAT	219	40.169	27.215	74.247	1.00	37.83	SOLV
HETATM 3206	OH2 WAT	220	38.737	39.516	73.171	1.00	49.20	SOLV
HETATM 3207	OH2 WAT	221	50.628	21.408	46.879	1.00	45.57	SOLV
HETATM 3208	OH2 WAT	222	35.436	43.288	75.660	1.00	37.33	SOLV
HETATM 3209	OH2 WAT	223	34.390	16.963	55.285	1.00	35.10	SOLV
HETATM 3210	OH2 WAT	224	21.800	35.454	34.475	1.00	46.29	SOLV
HETATM 3211	OH2 WAT	225	15.751	40.989	46.787	1.00	62.75	SOLV
HETATM 3212	OH2 WAT	226	23.844	48.662	66.295	1.00	38.35	SOLV
HETATM 3213	OH2 WAT	227	47.225	20.562	55.117	1.00	49.99	SOLV
HETATM 3214	OH2 WAT	228	23.426	19.272	50.565	1.00	30.07	SOLV

68/263

Figure 17-1

					Residue #	X	Y	Z	OCC.	B	Segment ID
ATOM	1	CB	ALA	A	2	43.739	36.862	75.052	1.00	64.01	6
ATOM	2	C	ALA	A	2	44.405	38.106	72.971	1.00	60.02	6
ATOM	3	O	ALA	A	2	43.251	38.536	72.908	1.00	57.94	8
ATOM	4	N	ALA	A	2	46.142	37.179	74.497	1.00	62.88	7
ATOM	5	CA	ALA	A	2	44.776	36.966	73.923	1.00	63.02	6
ATOM	6	N	LYS	A	3	45.398	38.588	72.233	1.00	55.40	7
ATOM	7	CA	LYS	A	3	45.196	39.671	71.287	1.00	53.02	6
ATOM	8	CB	LYS	A	3	46.443	39.830	70.421	1.00	53.11	6
ATOM	9	CG	LYS	A	3	47.703	40.093	71.217	1.00	57.36	6
ATOM	10	CD	LYS	A	3	48.941	39.976	70.349	1.00	60.94	6
ATOM	11	CE	LYS	A	3	48.909	40.957	69.196	1.00	63.48	6
ATOM	12	NZ	LYS	A	3	50.075	40.765	68.294	1.00	66.87	7
ATOM	13	C	LYS	A	3	43.986	39.401	70.399	1.00	50.49	6
ATOM	14	O	LYS	A	3	43.691	38.255	70.063	1.00	52.50	8
ATOM	15	N	VAL	A	4	43.281	40.464	70.034	1.00	45.96	7
ATOM	16	CA	VAL	A	4	42.122	40.352	69.167	1.00	41.16	6
ATOM	17	CB	VAL	A	4	40.983	41.272	69.638	1.00	41.53	6
ATOM	18	CG1	VAL	A	4	39.734	41.028	68.797	1.00	40.07	6
ATOM	19	CG2	VAL	A	4	40.705	41.033	71.115	1.00	38.31	6
ATOM	20	C	VAL	A	4	42.619	40.796	67.796	1.00	39.96	6
ATOM	21	O	VAL	A	4	43.123	41.914	67.645	1.00	39.15	8
ATOM	22	N	LYS	A	5	42.486	39.916	66.807	1.00	36.24	7
ATOM	23	CA	LYS	A	5	42.956	40.186	65.449	1.00	35.66	6
ATOM	24	CB	LYS	A	5	43.930	39.088	65.024	1.00	37.33	6
ATOM	25	CG	LYS	A	5	45.197	38.978	65.860	1.00	38.24	6
ATOM	26	CD	LYS	A	5	46.113	40.179	65.659	1.00	35.41	6
ATOM	27	CE	LYS	A	5	47.436	39.957	66.369	1.00	37.46	6
ATOM	28	NZ	LYS	A	5	48.345	41.121	66.245	1.00	35.63	7
ATOM	29	C	LYS	A	5	41.840	40.254	64.415	1.00	34.40	6
ATOM	30	O	LYS	A	5	40.788	39.641	64.588	1.00	33.92	8
ATOM	31	N	LEU	A	6	42.082	40.983	63.329	1.00	32.52	7
ATOM	32	CA	LEU	A	6	41.097	41.094	62.253	1.00	33.64	6
ATOM	33	CB	LEU	A	6	40.589	42.532	62.114	1.00	31.83	6
ATOM	34	CG	LEU	A	6	39.346	42.823	61.248	1.00	32.93	6
ATOM	35	CD1	LEU	A	6	39.356	44.295	60.899	1.00	28.95	6
ATOM	36	CD2	LEU	A	6	39.336	42.031	59.964	1.00	32.87	6
ATOM	37	C	LEU	A	6	41.802	40.721	60.955	1.00	35.09	6
ATOM	38	O	LEU	A	6	42.631	41.491	60.468	1.00	36.93	8
ATOM	39	N	ILE	A	7	41.494	39.561	60.382	1.00	35.52	7
ATOM	40	CA	ILE	A	7	42.145	39.199	59.129	1.00	35.14	6
ATOM	41	CB	ILE	A	7	42.062	37.711	58.850	1.00	33.68	6
ATOM	42	CG2	ILE	A	7	42.731	37.409	57.517	1.00	32.87	6
ATOM	43	CG1	ILE	A	7	42.746	36.941	59.975	1.00	33.32	6
ATOM	44	CD1	ILE	A	7	42.744	35.451	59.755	1.00	35.09	6
ATOM	45	C	ILE	A	7	41.487	39.935	57.971	1.00	37.13	6
ATOM	46	O	ILE	A	7	40.258	39.933	57.855	1.00	35.21	8
ATOM	47	N	GLY	A	8	42.304	40.563	57.124	1.00	37.25	7
ATOM	48	CA	GLY	A	8	41.771	41.305	55.994	1.00	38.69	6
ATOM	49	C	GLY	A	8	42.809	41.939	55.079	1.00	39.73	6
ATOM	50	O	GLY	A	8	44.015	41.827	55.321	1.00	39.21	8
ATOM	51	N	THR	A	9	42.335	42.622	54.033	1.00	39.41	7
ATOM	52	CA	THR	A	9	43.212	43.268	53.057	1.00	38.69	6
ATOM	53	CB	THR	A	9	44.132	42.210	52.390	1.00	37.27	6
ATOM	54	CG1	THR	A	9	44.754	42.771	51.230	1.00	36.82	8
ATOM	55	CG2	THR	A	9	43.332	40.972	52.001	1.00	38.59	6
ATOM	56	C	THR	A	9	42.447	44.045	51.970	1.00	38.60	6
ATOM	57	O	THR	A	9	41.434	43.569	51.452	1.00	37.30	8
ATOM	58	N	LEU	A	10	42.939	45.238	51.628	1.00	38.14	7
ATOM	59	CA	LEU	A	10	42.304	46.077	50.609	1.00	39.39	6
ATOM	60	CB	LEU	A	10	43.026	47.418	50.456	1.00	38.98	6
ATOM	61	CG	LEU	A	10	42.836	48.506	51.510	1.00	39.68	6
ATOM	62	CD1	LEU	A	10	41.343	48.830	51.594	1.00	40.22	6
ATOM	63	CD2	LEU	A	10	43.382	48.057	52.857	1.00	40.11	6
ATOM	64	C	LEU	A	10	42.238	45.432	49.239	1.00	41.66	6
ATOM	65	O	LEU	A	10	41.462	45.863	48.381	1.00	42.08	8
ATOM	66	N	ASP	A	11	43.052	44.408	49.025	1.00	43.51	7

69/263

Figure 17-2

ATOM	67	CA	ASP	A	11	43.071	43.731	47.737	1.00	47.27	6
ATOM	68	CB	ASP	A	11	44.250	42.765	47.694	1.00	51.03	6
ATOM	69	CG	ASP	A	11	45.579	43.479	47.858	1.00	54.10	6
ATOM	70	OD1	ASP	A	11	45.944	44.282	46.975	1.00	55.93	8
ATOM	71	OD2	ASP	A	11	46.255	43.251	48.879	1.00	57.79	8
ATOM	72	C	ASP	A	11	41.756	43.016	47.423	1.00	46.36	6
ATOM	73	O	ASP	A	11	41.472	42.702	46.266	1.00	43.49	8
ATOM	74	N	TYR	A	12	40.954	42.767	48.456	1.00	46.80	7
ATOM	75	CA	TYR	A	12	39.654	42.116	48.284	1.00	45.92	6
ATOM	76	CB	TYR	A	12	38.953	41.942	49.638	1.00	41.38	6
ATOM	77	CG	TYR	A	12	39.358	40.697	50.390	1.00	38.82	6
ATOM	78	CD1	TYR	A	12	39.531	40.720	51.775	1.00	37.95	6
ATOM	79	CE1	TYR	A	12	39.869	39.560	52.476	1.00	36.18	6
ATOM	80	CD2	TYR	A	12	39.533	39.479	49.721	1.00	37.69	6
ATOM	81	CE2	TYR	A	12	39.868	38.316	50.415	1.00	35.83	6
ATOM	82	CZ	TYR	A	12	40.032	38.365	51.787	1.00	34.10	6
ATOM	83	OH	TYR	A	12	40.339	37.216	52.470	1.00	36.31	8
ATOM	84	C	TYR	A	12	38.786	42.966	47.378	1.00	46.56	6
ATOM	85	O	TYR	A	12	37.821	42.476	46.791	1.00	47.38	8
ATOM	86	N	GLY	A	13	39.138	44.247	47.278	1.00	47.28	7
ATOM	87	CA	GLY	A	13	38.385	45.164	46.442	1.00	46.53	6
ATOM	88	C	GLY	A	13	38.650	44.934	44.968	1.00	45.60	6
ATOM	89	O	GLY	A	13	37.895	45.401	44.117	1.00	43.68	8
ATOM	90	N	LYS	A	14	39.725	44.210	44.672	1.00	46.52	7
ATOM	91	CA	LYS	A	14	40.112	43.908	43.296	1.00	47.28	6
ATOM	92	CB	LYS	A	14	41.629	43.748	43.201	1.00	50.22	6
ATOM	93	CG	LYS	A	14	42.396	45.044	43.307	1.00	57.12	6
ATOM	94	CD	LYS	A	14	42.038	46.004	42.161	1.00	63.60	6
ATOM	95	CE	LYS	A	14	42.349	45.422	40.768	1.00	66.65	6
ATOM	96	NZ	LYS	A	14	41.529	44.220	40.387	1.00	67.70	7
ATOM	97	C	LYS	A	14	39.460	42.643	42.769	1.00	44.18	6
ATOM	98	O	LYS	A	14	39.564	42.325	41.585	1.00	40.33	8
ATOM	99	N	TYR	A	15	38.790	41.926	43.661	1.00	43.25	7
ATOM	100	CA	TYR	A	15	38.145	40.665	43.317	1.00	43.18	6
ATOM	101	CB	TYR	A	15	38.789	39.547	44.142	1.00	36.88	6
ATOM	102	CG	TYR	A	15	40.302	39.560	44.053	1.00	32.96	6
ATOM	103	CD1	TYR	A	15	41.084	39.107	45.108	1.00	30.90	6
ATOM	104	CE1	TYR	A	15	42.476	39.144	45.035	1.00	30.94	6
ATOM	105	CD2	TYR	A	15	40.952	40.049	42.912	1.00	33.01	6
ATOM	106	CE2	TYR	A	15	42.341	40.092	42.826	1.00	29.68	6
ATOM	107	CZ	TYR	A	15	43.098	39.639	43.890	1.00	30.99	6
ATOM	108	OH	TYR	A	15	44.471	39.673	43.809	1.00	28.02	8
ATOM	109	C	TYR	A	15	36.661	40.778	43.621	1.00	45.56	6
ATOM	110	O	TYR	A	15	36.149	40.153	44.552	1.00	45.22	8
ATOM	111	N	ARG	A	16	35.981	41.599	42.830	1.00	48.81	7
ATOM	112	CA	ARG	A	16	34.553	41.819	42.999	1.00	53.22	6
ATOM	113	CB	ARG	A	16	34.193	43.263	42.654	1.00	57.11	6
ATOM	114	CG	ARG	A	16	34.852	44.330	43.490	1.00	61.66	6
ATOM	115	CD	ARG	A	16	34.280	44.408	44.886	1.00	67.04	6
ATOM	116	NE	ARG	A	16	34.798	45.590	45.569	1.00	73.59	7
ATOM	117	CZ	ARG	A	16	34.612	46.837	45.141	1.00	75.03	6
ATOM	118	NH1	ARG	A	16	33.917	47.065	44.033	1.00	73.03	7
ATOM	119	NH2	ARG	A	16	35.142	47.856	45.808	1.00	75.79	7
ATOM	120	C	ARG	A	16	33.757	40.903	42.080	1.00	51.79	6
ATOM	121	O	ARG	A	16	34.192	40.593	40.970	1.00	50.89	8
ATOM	122	N	TYR	A	17	32.596	40.463	42.552	1.00	50.19	7
ATOM	123	CA	TYR	A	17	31.737	39.634	41.733	1.00	49.60	6
ATOM	124	CB	TYR	A	17	30.534	39.119	42.528	1.00	45.80	6
ATOM	125	CG	TYR	A	17	30.803	37.894	43.365	1.00	42.01	6
ATOM	126	CD1	TYR	A	17	31.589	37.932	44.438	1.00	42.45	6
ATOM	127	CE1	TYR	A	17	31.960	36.780	45.193	1.00	43.36	6
ATOM	128	CD2	TYR	A	17	30.185	36.680	43.062	1.00	39.89	6
ATOM	129	CE2	TYR	A	17	30.443	35.526	43.803	1.00	40.56	6
ATOM	130	CZ	TYR	A	17	31.333	35.578	44.869	1.00	41.98	6
ATOM	131	OH	TYR	A	17	31.600	34.438	45.598	1.00	34.66	8
ATOM	132	C	TYR	A	17	31.245	40.547	40.622	1.00	51.88	6

70/263

Figure 17-3

ATOM	133	O	TYR	A	17	31.332	41.772	40.726	1.00	47.86	8
ATOM	134	N	PRO	A	18	30.730	39.964	39.534	1.00	54.38	7
ATOM	135	CD	PRO	A	18	30.548	38.545	39.190	1.00	54.21	6
ATOM	136	CA	PRO	A	18	30.243	40.809	38.449	1.00	56.43	6
ATOM	137	CB	PRO	A	18	29.601	39.792	37.496	1.00	56.84	6
ATOM	138	CG	PRO	A	18	29.260	38.613	38.426	1.00	56.46	6
ATOM	139	C	PRO	A	18	29.273	41.891	38.932	1.00	58.74	6
ATOM	140	O	PRO	A	18	28.791	41.861	40.066	1.00	55.72	8
ATOM	141	N	LYS	A	19	29.017	42.851	38.052	1.00	62.10	7
ATOM	142	CA	LYS	A	19	28.127	43.973	38.314	1.00	64.85	6
ATOM	143	CB	LYS	A	19	27.972	44.761	37.022	1.00	69.74	6
ATOM	144	CG	LYS	A	19	28.008	43.925	35.740	1.00	74.99	6
ATOM	145	CD	LYS	A	19	26.895	42.881	35.668	1.00	78.18	6
ATOM	146	CE	LYS	A	19	26.981	42.010	34.420	1.00	80.24	6
ATOM	147	NZ	LYS	A	19	25.867	41.010	34.361	1.00	81.13	7
ATOM	148	C	LYS	A	19	26.750	43.619	38.869	1.00	64.77	6
ATOM	149	O	LYS	A	19	26.414	43.961	40.001	1.00	66.50	8
ATOM	150	N	ASN	A	20	25.957	42.933	38.062	1.00	63.75	7
ATOM	151	CA	ASN	A	20	24.612	42.556	38.439	1.00	62.96	6
ATOM	152	CB	ASN	A	20	23.870	42.031	37.208	1.00	67.42	6
ATOM	153	CG	ASN	A	20	22.392	41.833	37.459	1.00	72.29	6
ATOM	154	OD1	ASN	A	20	21.666	42.785	37.772	1.00	75.25	8
ATOM	155	ND2	ASN	A	20	21.931	40.594	37.322	1.00	74.38	7
ATOM	156	C	ASN	A	20	24.602	41.512	39.547	1.00	61.30	6
ATOM	157	O	ASN	A	20	23.629	40.773	39.698	1.00	61.49	8
ATOM	158	N	HIS	A	21	25.681	41.444	40.321	1.00	57.30	7
ATOM	159	CA	HIS	A	21	25.755	40.480	41.418	1.00	54.68	6
ATOM	160	CB	HIS	A	21	27.071	39.700	41.373	1.00	52.63	6
ATOM	161	CG	HIS	A	21	27.058	38.449	42.195	1.00	49.39	6
ATOM	162	CD2	HIS	A	21	27.336	38.236	43.503	1.00	49.39	6
ATOM	163	ND1	HIS	A	21	26.664	37.229	41.686	1.00	48.27	7
ATOM	164	CE1	HIS	A	21	26.704	36.320	42.643	1.00	48.16	6
ATOM	165	NE2	HIS	A	21	27.108	36.905	43.757	1.00	47.33	7
ATOM	166	C	HIS	A	21	25.664	41.215	42.760	1.00	52.89	6
ATOM	167	O	HIS	A	21	26.295	42.256	42.947	1.00	52.52	8
ATOM	168	N	PRO	A	22	24.880	40.679	43.713	1.00	50.81	7
ATOM	169	CD	PRO	A	22	24.076	39.444	43.661	1.00	48.50	6
ATOM	170	CA	PRO	A	22	24.734	41.310	45.029	1.00	48.02	6
ATOM	171	CB	PRO	A	22	23.860	40.308	45.783	1.00	47.45	6
ATOM	172	CG	PRO	A	22	22.990	39.754	44.667	1.00	47.76	6
ATOM	173	C	PRO	A	22	26.074	41.558	45.727	1.00	46.48	6
ATOM	174	O	PRO	A	22	26.164	42.405	46.615	1.00	45.69	8
ATOM	175	N	LEU	A	23	27.107	40.816	45.318	1.00	44.97	7
ATOM	176	CA	LEU	A	23	28.441	40.949	45.906	1.00	41.31	6
ATOM	177	CB	LEU	A	23	29.076	39.569	46.131	1.00	39.22	6
ATOM	178	CG	LEU	A	23	28.264	38.561	46.953	1.00	37.71	6
ATOM	179	CD1	LEU	A	23	29.075	37.288	47.157	1.00	35.07	6
ATOM	180	CD2	LEU	A	23	27.896	39.165	48.292	1.00	36.90	6
ATOM	181	C	LEU	A	23	29.334	41.789	45.003	1.00	40.14	6
ATOM	182	O	LEU	A	23	30.556	41.614	44.951	1.00	39.00	8
ATOM	183	N	LYS	A	24	28.706	42.705	44.284	1.00	39.67	7
ATOM	184	CA	LYS	A	24	29.430	43.590	43.398	1.00	42.88	6
ATOM	185	CB	LYS	A	24	28.480	44.120	42.323	1.00	40.24	6
ATOM	186	CG	LYS	A	24	28.949	45.362	41.610	1.00	44.08	6
ATOM	187	CD	LYS	A	24	28.247	46.600	42.166	1.00	44.47	6
ATOM	188	CE	LYS	A	24	26.732	46.492	41.968	1.00	43.23	6
ATOM	189	NZ	LYS	A	24	25.989	47.717	42.362	1.00	39.79	7
ATOM	190	C	LYS	A	24	30.031	44.723	44.217	1.00	43.70	6
ATOM	191	O	LYS	A	24	31.027	45.332	43.817	1.00	47.22	8
ATOM	192	N	ILE	A	25	29.431	44.976	45.378	1.00	42.27	7
ATOM	193	CA	ILE	A	25	29.870	46.035	46.289	1.00	39.86	6
ATOM	194	CB	ILE	A	25	28.763	46.407	47.306	1.00	37.72	6
ATOM	195	CG2	ILE	A	25	27.539	46.953	46.580	1.00	39.67	6
ATOM	196	CG1	ILE	A	25	28.410	45.168	48.145	1.00	35.25	6
ATOM	197	CD1	ILE	A	25	27.301	45.368	49.151	1.00	31.74	6
ATOM	198	C	ILE	A	25	31.078	45.625	47.112	1.00	40.23	6

71/263

Figure 17-4

ATOM	199	O	ILE	A	25	31.419	44.441	47.198	1.00	38.90	8
ATOM	200	N	PRO	A	26	31.762	46.616	47.709	1.00	40.18	7
ATOM	201	CD	PRO	A	26	31.523	48.051	47.533	1.00	40.58	6
ATOM	202	CA	PRO	A	26	32.939	46.437	48.558	1.00	38.31	6
ATOM	203	CB	PRO	A	26	33.478	47.860	48.688	1.00	37.14	6
ATOM	204	CG	PRO	A	26	32.940	48.537	47.458	1.00	38.77	6
ATOM	205	C	PRO	A	26	32.433	45.903	49.891	1.00	37.32	6
ATOM	206	O	PRO	A	26	31.416	46.372	50.412	1.00	32.70	8
ATOM	207	N	ARG	A	27	33.134	44.930	50.452	1.00	36.54	7
ATOM	208	CA	ARG	A	27	32.685	44.359	51.711	1.00	37.39	6
ATOM	209	CB	ARG	A	27	32.116	42.952	51.455	1.00	35.29	6
ATOM	210	CG	ARG	A	27	31.047	42.956	50.355	1.00	32.69	6
ATOM	211	CD	ARG	A	27	30.507	41.573	49.956	1.00	33.87	6
ATOM	212	NE	ARG	A	27	29.757	40.909	51.021	1.00	36.16	7
ATOM	213	CZ	ARG	A	27	30.293	40.132	51.959	1.00	37.11	6
ATOM	214	NH1	ARG	A	27	31.604	39.903	51.976	1.00	34.42	7
ATOM	215	NH2	ARG	A	27	29.516	39.597	52.896	1.00	33.67	7
ATOM	216	C	ARG	A	27	33.813	44.329	52.732	1.00	36.35	6
ATOM	217	O	ARG	A	27	33.881	45.188	53.610	1.00	35.77	8
ATOM	218	N	VAL	A	28	34.703	43.351	52.607	1.00	34.93	7
ATOM	219	CA	VAL	A	28	35.810	43.230	53.537	1.00	34.00	6
ATOM	220	CB	VAL	A	28	36.633	41.954	53.252	1.00	36.21	6
ATOM	221	CG1	VAL	A	28	37.574	41.652	54.424	1.00	33.59	6
ATOM	222	CG2	VAL	A	28	35.696	40.790	52.992	1.00	37.05	6
ATOM	223	C	VAL	A	28	36.712	44.454	53.423	1.00	31.91	6
ATOM	224	O	VAL	A	28	37.216	44.959	54.427	1.00	31.45	8
ATOM	225	N	SER	A	29	36.908	44.936	52.199	1.00	33.12	7
ATOM	226	CA	SER	A	29	37.751	46.111	51.967	1.00	32.03	6
ATOM	227	CB	SER	A	29	38.205	46.181	50.499	1.00	31.77	6
ATOM	228	OG	SER	A	29	37.113	46.223	49.600	1.00	30.80	8
ATOM	229	C	SER	A	29	37.003	47.380	52.353	1.00	30.16	6
ATOM	230	O	SER	A	29	37.604	48.404	52.650	1.00	28.70	8
ATOM	231	N	LEU	A	30	35.682	47.310	52.352	1.00	32.43	7
ATOM	232	CA	LEU	A	30	34.900	48.465	52.745	1.00	34.56	6
ATOM	233	CB	LEU	A	30	33.463	48.358	52.221	1.00	36.44	6
ATOM	234	CG	LEU	A	30	32.508	49.513	52.560	1.00	36.79	6
ATOM	235	CD1	LEU	A	30	32.070	49.446	54.012	1.00	36.73	6
ATOM	236	CD2	LEU	A	30	33.202	50.840	52.256	1.00	37.84	6
ATOM	237	C	LEU	A	30	34.902	48.527	54.262	1.00	34.89	6
ATOM	238	O	LEU	A	30	35.033	49.601	54.841	1.00	37.58	8
ATOM	239	N	LEU	A	31	34.761	47.366	54.897	1.00	34.07	7
ATOM	240	CA	LEU	A	31	34.743	47.276	56.350	1.00	34.85	6
ATOM	241	CB	LEU	A	31	34.768	45.808	56.791	1.00	36.37	6
ATOM	242	CG	LEU	A	31	34.459	45.471	58.261	1.00	36.04	6
ATOM	243	CD1	LEU	A	31	34.841	44.027	58.532	1.00	35.13	6
ATOM	244	CD2	LEU	A	31	35.228	46.357	59.194	1.00	35.86	6
ATOM	245	C	LEU	A	31	35.976	47.994	56.894	1.00	36.43	6
ATOM	246	O	LEU	A	31	35.855	49.035	57.544	1.00	35.87	8
ATOM	247	N	LEU	A	32	37.157	47.426	56.635	1.00	37.76	7
ATOM	248	CA	LEU	A	32	38.420	48.015	57.087	1.00	36.82	6
ATOM	249	CB	LEU	A	32	39.611	47.318	56.418	1.00	36.37	6
ATOM	250	CG	LEU	A	32	40.030	45.888	56.774	1.00	39.11	6
ATOM	251	CD1	LEU	A	32	41.117	45.420	55.815	1.00	35.16	6
ATOM	252	CD2	LEU	A	32	40.538	45.830	58.214	1.00	37.73	6
ATOM	253	C	LEU	A	32	38.500	49.513	56.780	1.00	34.84	6
ATOM	254	O	LEU	A	32	38.846	50.326	57.644	1.00	36.58	8
ATOM	255	N	ARG	A	33	38.184	49.877	55.545	1.00	31.37	7
ATOM	256	CA	ARG	A	33	38.247	51.270	55.150	1.00	32.53	6
ATOM	257	CB	ARG	A	33	37.927	51.398	53.662	1.00	31.52	6
ATOM	258	CG	ARG	A	33	38.481	52.652	53.042	1.00	35.88	6
ATOM	259	CD	ARG	A	33	38.107	52.752	51.581	1.00	43.44	6
ATOM	260	NE	ARG	A	33	38.521	51.583	50.811	1.00	48.37	7
ATOM	261	CZ	ARG	A	33	38.348	51.469	49.497	1.00	52.27	6
ATOM	262	NH1	ARG	A	33	37.771	52.459	48.823	1.00	51.75	7
ATOM	263	NH2	ARG	A	33	38.739	50.369	48.858	1.00	51.08	7
ATOM	264	C	ARG	A	33	37.274	52.102	55.989	1.00	32.32	6

72/263

Figure 17-5

ATOM	265	O	ARG	A	33	37.471	53.299	56.196	1.00	29.23	8
ATOM	266	N	PHE	A	34	36.231	51.445	56.484	1.00	32.58	7
ATOM	267	CA	PHE	A	34	35.216	52.096	57.304	1.00	32.69	6
ATOM	268	CB	PHE	A	34	33.952	51.232	57.359	1.00	31.22	6
ATOM	269	CG	PHE	A	34	32.838	51.825	58.183	1.00	28.74	6
ATOM	270	CD1	PHE	A	34	32.085	52.688	57.700	1.00	22.76	6
ATOM	271	CD2	PHE	A	34	32.551	51.322	59.456	1.00	28.09	6
ATOM	272	CE1	PHE	A	34	31.061	53.441	58.472	1.00	23.70	6
ATOM	273	CE2	PHE	A	34	31.524	51.873	60.235	1.00	24.59	6
ATOM	274	CZ	PHE	A	34	30.781	52.929	59.741	1.00	21.39	6
ATOM	275	C	PHE	A	34	35.734	52.319	58.719	1.00	33.45	6
ATOM	276	O	PHE	A	34	35.635	53.425	59.258	1.00	35.49	8
ATOM	277	N	LYS	A	35	36.276	51.264	59.323	1.00	34.52	7
ATOM	278	CA	LYS	A	35	36.805	51.360	60.678	1.00	36.51	6
ATOM	279	CB	LYS	A	35	37.118	49.977	61.235	1.00	36.47	6
ATOM	280	CG	LYS	A	35	35.912	49.074	61.343	1.00	40.81	6
ATOM	281	CD	LYS	A	35	36.246	47.801	62.090	1.00	44.10	6
ATOM	282	CE	LYS	A	35	37.347	47.029	61.402	1.00	47.46	6
ATOM	283	NZ	LYS	A	35	38.601	47.823	61.276	1.00	53.53	7
ATOM	284	C	LYS	A	35	38.054	52.222	60.735	1.00	36.61	6
ATOM	285	O	LYS	A	35	38.352	52.824	61.766	1.00	36.78	8
ATOM	286	N	ASP	A	36	38.794	52.267	59.635	1.00	36.27	7
ATOM	287	CA	ASP	A	36	39.980	53.090	59.592	1.00	39.71	6
ATOM	288	CB	ASP	A	36	40.679	52.937	58.239	1.00	44.78	6
ATOM	289	CG	ASP	A	36	41.863	53.892	58.075	1.00	47.10	6
ATOM	290	OD1	ASP	A	36	42.803	53.352	58.906	1.00	44.02	8
ATOM	291	OD2	ASP	A	36	41.843	54.682	57.106	1.00	48.43	8
ATOM	292	C	ASP	A	36	39.508	54.530	59.789	1.00	39.99	6
ATOM	293	O	ASP	A	36	40.023	55.258	60.636	1.00	40.76	8
ATOM	294	N	ALA	A	37	38.506	54.919	59.007	1.00	38.59	7
ATOM	295	CA	ALA	A	37	37.939	56.258	59.066	1.00	37.14	6
ATOM	296	CB	ALA	A	37	36.857	56.402	58.000	1.00	35.85	6
ATOM	297	C	ALA	A	37	37.354	56.549	60.446	1.00	38.34	6
ATOM	298	O	ALA	A	37	37.391	57.687	60.928	1.00	37.32	8
ATOM	299	N	MET	A	38	36.809	55.518	61.079	1.00	36.19	7
ATOM	300	CA	MET	A	38	36.213	55.674	62.397	1.00	36.80	6
ATOM	301	CB	MET	A	38	35.141	54.598	62.606	1.00	37.38	6
ATOM	302	CG	MET	A	38	33.938	54.717	61.673	1.00	37.60	6
ATOM	303	SD	MET	A	38	32.887	56.165	61.999	1.00	33.61	16
ATOM	304	CE	MET	A	38	32.398	55.824	63.680	1.00	35.60	6
ATOM	305	C	MET	A	38	37.262	55.582	63.502	1.00	35.84	6
ATOM	306	O	MET	A	38	36.937	55.688	64.692	1.00	34.89	8
ATOM	307	N	ASN	A	39	38.518	55.400	63.100	1.00	33.83	7
ATOM	308	CA	ASN	A	39	39.626	55.264	64.044	1.00	34.94	6
ATOM	309	CB	ASN	A	39	39.897	56.582	64.775	1.00	32.48	6
ATOM	310	CG	ASN	A	39	40.213	57.717	63.825	1.00	32.34	6
ATOM	311	OD1	ASN	A	39	41.128	57.621	63.009	1.00	31.85	8
ATOM	312	ND2	ASN	A	39	39.455	58.800	63.924	1.00	30.92	7
ATOM	313	C	ASN	A	39	39.253	54.183	65.045	1.00	36.87	6
ATOM	314	O	ASN	A	39	39.403	54.357	66.260	1.00	36.60	8
ATOM	315	N	LEU	A	40	38.752	53.067	64.518	1.00	37.48	7
ATOM	316	CA	LEU	A	40	38.341	51.933	65.336	1.00	39.66	6
ATOM	317	CB	LEU	A	40	36.863	51.622	65.086	1.00	41.35	6
ATOM	318	CG	LEU	A	40	35.858	52.712	65.476	1.00	42.69	6
ATOM	319	CD1	LEU	A	40	34.448	52.261	65.111	1.00	45.05	6
ATOM	320	CD2	LEU	A	40	35.951	52.989	66.966	1.00	39.44	6
ATOM	321	C	LEU	A	40	39.184	50.687	65.058	1.00	39.79	6
ATOM	322	O	LEU	A	40	38.804	49.575	65.434	1.00	36.88	8
ATOM	323	N	ILE	A	41	40.337	50.889	64.420	1.00	40.50	7
ATOM	324	CA	ILE	A	41	41.237	49.790	64.068	1.00	41.39	6
ATOM	325	CB	ILE	A	41	40.780	49.141	62.724	1.00	39.24	6
ATOM	326	CG2	ILE	A	41	41.017	50.103	61.564	1.00	36.97	6
ATOM	327	CG1	ILE	A	41	41.513	47.824	62.482	1.00	36.76	6
ATOM	328	CD1	ILE	A	41	41.085	46.715	63.403	1.00	35.59	6
ATOM	329	C	ILE	A	41	42.684	50.295	63.913	1.00	44.37	6
ATOM	330	O	ILE	A	41	42.927	51.328	63.277	1.00	46.01	8

ATOM	331	N	ASP	A	42	43.646	49.582	64.497	1.00	45.19	7
ATOM	332	CA	ASP	A	42	45.049	49.982	64.372	1.00	45.62	6
ATOM	333	CB	ASP	A	42	45.716	50.090	65.742	1.00	45.17	6
ATOM	334	CG	ASP	A	42	44.966	51.005	66.682	1.00	44.43	6
ATOM	335	OD1	ASP	A	42	44.731	52.177	66.322	1.00	39.84	8
ATOM	336	OD2	ASP	A	42	44.612	50.546	67.787	1.00	48.50	8
ATOM	337	C	ASP	A	42	45.750	48.915	63.551	1.00	48.47	6
ATOM	338	O	ASP	A	42	45.316	47.757	63.547	1.00	49.85	8
ATOM	339	N	GLU	A	43	46.830	49.288	62.864	1.00	49.24	7
ATOM	340	CA	GLU	A	43	47.553	48.325	62.028	1.00	50.79	6
ATOM	341	CB	GLU	A	43	48.820	48.956	61.431	1.00	49.90	6
ATOM	342	CG	GLU	A	43	48.544	50.029	60.378	1.00	57.20	6
ATOM	343	CD	GLU	A	43	49.808	50.537	59.690	1.00	59.56	6
ATOM	344	OE1	GLU	A	43	50.517	49.721	59.061	1.00	65.05	8
ATOM	345	OE2	GLU	A	43	50.095	51.750	59.772	1.00	57.82	8
ATOM	346	C	GLU	A	43	47.918	47.020	62.733	1.00	49.73	6
ATOM	347	O	GLU	A	43	47.813	45.943	62.149	1.00	49.18	8
ATOM	348	N	LYS	A	44	48.324	47.118	63.992	1.00	49.40	7
ATOM	349	CA	LYS	A	44	48.730	45.949	64.762	1.00	49.09	6
ATOM	350	CB	LYS	A	44	49.317	46.418	66.093	1.00	52.46	6
ATOM	351	CG	LYS	A	44	50.448	47.421	65.899	1.00	55.75	6
ATOM	352	CD	LYS	A	44	51.167	47.749	67.201	1.00	58.74	6
ATOM	353	CE	LYS	A	44	52.327	48.704	66.949	1.00	58.48	6
ATOM	354	NZ	LYS	A	44	53.122	48.968	68.176	1.00	58.95	7
ATOM	355	C	LYS	A	44	47.638	44.897	64.994	1.00	47.63	6
ATOM	356	O	LYS	A	44	47.932	43.738	65.290	1.00	45.13	8
ATOM	357	N	GLU	A	45	46.379	45.298	64.854	1.00	45.25	7
ATOM	358	CA	GLU	A	45	45.268	44.374	65.046	1.00	43.09	6
ATOM	359	CB	GLU	A	45	44.024	45.143	65.514	1.00	41.19	6
ATOM	360	CG	GLU	A	45	44.192	45.859	66.844	1.00	36.83	6
ATOM	361	CD	GLU	A	45	43.003	46.741	67.204	1.00	38.92	6
ATOM	362	OE1	GLU	A	45	42.707	47.701	66.447	1.00	37.30	8
ATOM	363	OE2	GLU	A	45	42.368	46.479	68.253	1.00	36.33	8
ATOM	364	C	GLU	A	45	44.969	43.660	63.726	1.00	43.04	6
ATOM	365	O	GLU	A	45	44.480	42.523	63.699	1.00	45.03	8
ATOM	366	N	LEU	A	46	45.282	44.341	62.632	1.00	40.29	7
ATOM	367	CA	LEU	A	46	45.042	43.823	61.299	1.00	37.16	6
ATOM	368	CB	LEU	A	46	44.910	44.990	60.331	1.00	37.86	6
ATOM	369	CG	LEU	A	46	44.822	44.658	58.845	1.00	39.22	6
ATOM	370	CD1	LEU	A	46	43.655	43.726	58.563	1.00	40.68	6
ATOM	371	CD2	LEU	A	46	44.673	45.964	58.080	1.00	41.62	6
ATOM	372	C	LEU	A	46	46.090	42.860	60.774	1.00	36.54	6
ATOM	373	O	LEU	A	46	47.275	43.192	60.698	1.00	39.86	8
ATOM	374	N	ILE	A	47	45.646	41.662	60.406	1.00	33.49	7
ATOM	375	CA	ILE	A	47	46.540	40.657	59.844	1.00	30.51	6
ATOM	376	CB	ILE	A	47	46.333	39.253	60.491	1.00	34.31	6
ATOM	377	CG2	ILE	A	47	47.346	38.262	59.930	1.00	32.16	6
ATOM	378	CG1	ILE	A	47	46.504	39.328	62.010	1.00	32.65	6
ATOM	379	CD1	ILE	A	47	47.858	39.846	62.448	1.00	38.97	6
ATOM	380	C	ILE	A	47	46.196	40.570	58.362	1.00	28.36	6
ATOM	381	O	ILE	A	47	45.037	40.342	58.003	1.00	26.11	8
ATOM	382	N	LYS	A	48	47.194	40.772	57.504	1.00	27.77	7
ATOM	383	CA	LYS	A	48	46.985	40.713	56.056	1.00	25.80	6
ATOM	384	CB	LYS	A	48	48.258	41.087	55.308	1.00	23.91	6
ATOM	385	CG	LYS	A	48	48.056	41.273	53.811	1.00	24.90	6
ATOM	386	CD	LYS	A	48	49.389	41.352	53.091	1.00	26.39	6
ATOM	387	CE	LYS	A	48	49.233	41.864	51.679	1.00	27.71	6
ATOM	388	NZ	LYS	A	48	48.774	43.275	51.696	1.00	32.59	7
ATOM	389	C	LYS	A	48	46.595	39.299	55.654	1.00	26.32	6
ATOM	390	O	LYS	A	48	47.072	38.325	56.235	1.00	27.65	8
ATOM	391	N	SER	A	49	45.735	39.183	54.653	1.00	24.73	7
ATOM	392	CA	SER	A	49	45.299	37.876	54.205	1.00	27.36	6
ATOM	393	CB	SER	A	49	43.952	37.979	53.479	1.00	25.04	6
ATOM	394	CG	SER	A	49	42.911	38.329	54.373	1.00	26.94	8
ATOM	395	C	SER	A	49	46.322	37.211	53.293	1.00	28.97	6
ATOM	396	O	SER	A	49	47.095	37.885	52.612	1.00	31.89	8

74/263

Figure 17-7

ATOM	397	N	ARG	A	50	46.315	35.879	53.296	1.00	29.71	7
ATOM	398	CA	ARG	A	50	47.211	35.087	52.463	1.00	25.78	6
ATOM	399	CB	ARG	A	50	48.249	34.351	53.318	1.00	26.20	6
ATOM	400	CG	ARG	A	50	47.687	33.204	54.172	1.00	22.71	6
ATOM	401	CD	ARG	A	50	48.818	32.468	54.890	1.00	22.95	6
ATOM	402	NE	ARG	A	50	48.359	31.385	55.762	1.00	19.20	7
ATOM	403	CZ	ARG	A	50	47.708	30.306	55.345	1.00	16.85	6
ATOM	404	NH1	ARG	A	50	47.430	30.151	54.055	1.00	17.77	7
ATOM	405	NH2	ARG	A	50	47.334	29.385	56.223	1.00	14.56	7
ATOM	406	C	ARG	A	50	46.370	34.051	51.723	1.00	23.30	6
ATOM	407	O	ARG	A	50	45.319	33.635	52.206	1.00	16.92	8
ATOM	408	N	PRO	A	51	46.823	33.628	50.534	1.00	21.06	7
ATOM	409	CD	PRO	A	51	48.021	34.038	49.789	1.00	20.50	6
ATOM	410	CA	PRO	A	51	46.086	32.633	49.761	1.00	22.69	6
ATOM	411	CB	PRO	A	51	46.862	32.592	48.451	1.00	21.57	6
ATOM	412	CG	PRO	A	51	47.503	33.984	48.392	1.00	20.57	6
ATOM	413	C	PRO	A	51	46.153	31.300	50.498	1.00	26.71	6
ATOM	414	O	PRO	A	51	47.071	31.066	51.293	1.00	31.32	8
ATOM	415	N	ALA	A	52	45.176	30.435	50.250	1.00	26.02	7
ATOM	416	CA	ALA	A	52	45.151	29.121	50.876	1.00	25.76	6
ATOM	417	CB	ALA	A	52	43.720	28.585	50.933	1.00	21.42	6
ATOM	418	C	ALA	A	52	46.013	28.227	50.000	1.00	26.31	6
ATOM	419	O	ALA	A	52	45.878	28.239	48.780	1.00	30.31	8
ATOM	420	N	THR	A	53	46.909	27.464	50.608	1.00	26.80	7
ATOM	421	CA	THR	A	53	47.759	26.578	49.831	1.00	27.52	6
ATOM	422	CB	THR	A	53	48.845	25.975	50.717	1.00	26.27	6
ATOM	423	OG1	THR	A	53	48.255	25.053	51.641	1.00	29.51	8
ATOM	424	CG2	THR	A	53	49.522	27.076	51.502	1.00	24.66	6
ATOM	425	C	THR	A	53	46.908	25.462	49.209	1.00	26.58	6
ATOM	426	O	THR	A	53	45.778	25.228	49.634	1.00	21.98	8
ATOM	427	N	LYS	A	54	47.455	24.782	48.203	1.00	29.62	7
ATOM	428	CA	LYS	A	54	46.739	23.713	47.507	1.00	32.62	6
ATOM	429	CB	LYS	A	54	47.601	23.151	46.370	1.00	31.99	6
ATOM	430	CG	LYS	A	54	46.985	21.967	45.629	1.00	36.62	6
ATOM	431	CD	LYS	A	54	45.733	22.352	44.866	1.00	40.69	6
ATOM	432	CE	LYS	A	54	46.058	23.173	43.625	1.00	46.44	6
ATOM	433	NZ	LYS	A	54	46.844	22.393	42.614	1.00	50.68	7
ATOM	434	C	LYS	A	54	46.348	22.595	48.465	1.00	36.00	6
ATOM	435	O	LYS	A	54	45.277	21.991	48.330	1.00	34.77	8
ATOM	436	N	GLU	A	55	47.216	22.336	49.443	1.00	37.91	7
ATOM	437	CA	GLU	A	55	46.979	21.290	50.433	1.00	36.96	6
ATOM	438	CB	GLU	A	55	48.240	21.100	51.281	1.00	40.29	6
ATOM	439	CG	GLU	A	55	48.216	19.887	52.195	1.00	47.95	6
ATOM	440	CD	GLU	A	55	49.552	19.654	52.891	1.00	51.01	6
ATOM	441	OE1	GLU	A	55	49.659	18.688	53.679	1.00	52.65	8
ATOM	442	OE2	GLU	A	55	50.497	20.437	52.646	1.00	51.27	8
ATOM	443	C	GLU	A	55	45.771	21.609	51.322	1.00	34.10	6
ATOM	444	O	GLU	A	55	44.892	20.769	51.496	1.00	33.08	8
ATOM	445	N	GLU	A	56	45.723	22.827	51.866	1.00	32.39	7
ATOM	446	CA	GLU	A	56	44.621	23.256	52.733	1.00	30.13	6
ATOM	447	CB	GLU	A	56	44.824	24.714	53.177	1.00	25.28	6
ATOM	448	CG	GLU	A	56	46.204	24.994	53.758	1.00	28.82	6
ATOM	449	CD	GLU	A	56	46.421	26.450	54.181	1.00	30.74	6
ATOM	450	OE1	GLU	A	56	46.072	27.369	53.398	1.00	29.77	8
ATOM	451	OE2	GLU	A	56	46.969	26.674	55.288	1.00	25.98	8
ATOM	452	C	GLU	A	56	43.264	23.114	52.024	1.00	29.63	6
ATOM	453	O	GLU	A	56	42.299	22.584	52.595	1.00	29.90	8
ATOM	454	N	LEU	A	57	43.188	23.581	50.780	1.00	26.76	7
ATOM	455	CA	LEU	A	57	41.944	23.490	50.020	1.00	25.29	6
ATOM	456	CB	LEU	A	57	42.132	24.103	48.629	1.00	22.68	6
ATOM	457	CG	LEU	A	57	42.402	25.612	48.572	1.00	22.39	5
ATOM	458	CD1	LEU	A	57	42.654	26.045	47.123	1.00	20.77	6
ATOM	459	CD2	LEU	A	57	41.211	26.366	49.156	1.00	17.66	6
ATOM	460	C	LEU	A	57	41.479	22.037	49.896	1.00	26.02	6
ATOM	461	O	LEU	A	57	40.284	21.741	50.014	1.00	23.41	8
ATOM	462	N	LEU	A	58	42.444	21.143	49.675	1.00	24.82	7

75/263

Figure 17-8

ATOM	463	CA	LEU	A	58	42.194	19.718	49.526	1.00	22.44	6
ATOM	464	CB	LEU	A	58	43.434	19.027	48.965	1.00	21.02	6
ATOM	465	CG	LEU	A	58	43.838	19.471	47.558	1.00	22.94	6
ATOM	466	CD1	LEU	A	58	45.212	18.908	47.176	1.00	20.35	6
ATOM	467	CD2	LEU	A	58	42.755	19.033	46.587	1.00	23.28	6
ATOM	468	C	LEU	A	58	41.797	19.054	50.835	1.00	25.20	6
ATOM	469	O	LEU	A	58	41.456	17.867	50.854	1.00	26.55	8
ATOM	470	N	LEU	A	59	41.858	19.794	51.938	1.00	25.44	7
ATOM	471	CA	LEU	A	59	41.446	19.212	53.211	1.00	25.24	6
ATOM	472	CB	LEU	A	59	41.559	20.229	54.350	1.00	24.68	6
ATOM	473	CG	LEU	A	59	42.956	20.490	54.912	1.00	27.05	6
ATOM	474	CD1	LEU	A	59	42.912	21.565	56.001	1.00	24.76	6
ATOM	475	CD2	LEU	A	59	43.492	19.184	55.474	1.00	26.99	6
ATOM	476	C	LEU	A	59	39.991	18.807	53.045	1.00	24.22	6
ATOM	477	O	LEU	A	59	39.548	17.794	53.581	1.00	21.18	8
ATOM	478	N	PHE	A	60	39.270	19.615	52.270	1.00	25.00	7
ATOM	479	CA	PHE	A	60	37.859	19.403	52.011	1.00	25.00	6
ATOM	480	CB	PHE	A	60	37.054	20.560	52.605	1.00	26.34	6
ATOM	481	CG	PHE	A	60	35.600	20.555	52.223	1.00	29.37	6
ATOM	482	CD1	PHE	A	60	34.811	19.422	52.427	1.00	27.57	6
ATOM	483	CD2	PHE	A	60	35.015	21.692	51.661	1.00	27.33	6
ATOM	484	CE1	PHE	A	60	33.466	19.419	52.077	1.00	27.00	6
ATOM	485	CE2	PHE	A	60	33.670	21.699	51.306	1.00	28.08	6
ATOM	486	CZ	PHE	A	60	32.893	20.559	51.513	1.00	29.48	6
ATOM	487	C	PHE	A	60	37.506	19.214	50.538	1.00	27.78	6
ATOM	488	O	PHE	A	60	37.022	18.143	50.158	1.00	31.57	8
ATOM	489	N	HIS	A	61	37.734	20.220	49.696	1.00	26.76	7
ATOM	490	CA	HIS	A	61	37.376	20.056	48.287	1.00	28.84	6
ATOM	491	CB	HIS	A	61	37.365	21.405	47.561	1.00	27.76	6
ATOM	492	CG	HIS	A	61	36.385	22.396	48.117	1.00	30.54	6
ATOM	493	CD2	HIS	A	61	35.056	22.549	47.907	1.00	33.74	6
ATOM	494	ND1	HIS	A	61	36.750	23.401	48.987	1.00	34.02	7
ATOM	495	CE1	HIS	A	61	35.691	24.135	49.286	1.00	32.07	6
ATOM	496	NE2	HIS	A	61	34.649	23.638	48.644	1.00	34.10	7
ATOM	497	C	HIS	A	61	38.278	19.056	47.539	1.00	28.38	6
ATOM	498	O	HIS	A	61	39.287	18.604	48.072	1.00	25.81	8
ATOM	499	N	THR	A	62	37.895	18.705	46.310	1.00	32.88	7
ATOM	500	CA	THR	A	62	38.658	17.749	45.488	1.00	34.68	6
ATOM	501	CB	THR	A	62	37.715	16.739	44.778	1.00	34.36	6
ATOM	502	OG1	THR	A	62	36.942	17.415	43.778	1.00	34.81	8
ATOM	503	CG2	THR	A	62	36.759	16.112	45.778	1.00	34.33	6
ATOM	504	C	THR	A	62	39.485	18.454	44.408	1.00	35.60	6
ATOM	505	O	THR	A	62	39.017	19.418	43.790	1.00	30.85	8
ATOM	506	N	GLU	A	63	40.700	17.958	44.166	1.00	37.38	7
ATOM	507	CA	GLU	A	63	41.587	18.555	43.165	1.00	40.68	6
ATOM	508	CB	GLU	A	63	42.759	17.626	42.840	1.00	43.75	6
ATOM	509	CG	GLU	A	63	43.719	17.389	43.987	1.00	50.68	6
ATOM	510	CD	GLU	A	63	45.026	16.760	43.529	1.00	55.36	6
ATOM	511	OE1	GLU	A	63	45.789	17.441	42.808	1.00	53.03	8
ATOM	512	OE2	GLU	A	63	45.285	15.585	43.883	1.00	59.56	8
ATOM	513	C	GLU	A	63	40.894	18.939	41.860	1.00	39.26	6
ATOM	514	O	GLU	A	63	40.771	20.116	41.535	1.00	42.33	8
ATOM	515	N	ASP	A	64	40.453	17.948	41.102	1.00	37.07	7
ATOM	516	CA	ASP	A	64	39.782	18.224	39.845	1.00	36.98	6
ATOM	517	CB	ASP	A	64	38.957	17.000	39.426	1.00	42.19	6
ATOM	518	CG	ASP	A	64	38.037	16.501	40.533	1.00	47.66	6
ATOM	519	OD1	ASP	A	64	37.039	17.193	40.851	1.00	47.95	8
ATOM	520	OD2	ASP	A	64	38.325	15.413	41.091	1.00	50.07	8
ATOM	521	C	ASP	A	64	38.908	19.480	39.906	1.00	33.40	6
ATOM	522	O	ASP	A	64	38.927	20.293	38.986	1.00	33.64	8
ATOM	523	N	TYR	A	65	38.156	19.641	40.990	1.00	30.57	7
ATOM	524	CA	TYR	A	65	37.286	20.806	41.157	1.00	29.65	6
ATOM	525	CB	TYR	A	65	36.300	20.560	42.316	1.00	30.16	6
ATOM	526	CG	TYR	A	65	35.557	21.790	42.810	1.00	28.49	6
ATOM	527	CD1	TYR	A	65	34.791	22.572	41.944	1.00	30.25	6
ATOM	528	CE1	TYR	A	65	34.126	23.715	42.399	1.00	28.36	6

ATOM	529	CD2	TYR	A	65	35.638	22.181	44.150	1.00	28.28	6
ATOM	530	CE2	TYR	A	65	34.980	23.320	44.617	1.00	26.96	6
ATOM	531	CZ	TYR	A	65	34.227	24.082	43.740	1.00	29.79	6
ATOM	532	OH	TYR	A	65	33.568	25.201	44.207	1.00	28.53	8
ATOM	533	C	TYR	A	65	38.118	22.061	41.418	1.00	29.15	6
ATOM	534	O	TYR	A	65	37.860	23.128	40.857	1.00	30.45	8
ATOM	535	N	ILE	A	66	39.122	21.926	42.270	1.00	26.61	7
ATOM	536	CA	ILE	A	66	39.986	23.041	42.597	1.00	26.35	6
ATOM	537	CB	ILE	A	66	40.998	22.652	43.687	1.00	26.25	6
ATOM	538	CG2	ILE	A	66	42.009	23.753	43.869	1.00	21.20	6
ATOM	539	CG1	ILE	A	66	40.264	22.341	44.992	1.00	29.30	6
ATOM	540	CD1	ILE	A	66	39.478	23.517	45.555	1.00	30.52	6
ATOM	541	C	ILE	A	66	40.761	23.504	41.381	1.00	28.07	6
ATOM	542	O	ILE	A	66	41.039	24.696	41.225	1.00	31.26	8
ATOM	543	N	ASN	A	67	41.125	22.559	40.521	1.00	28.47	7
ATOM	544	CA	ASN	A	67	41.902	22.898	39.337	1.00	30.15	6
ATOM	545	CB	ASN	A	67	42.563	21.656	38.726	1.00	34.20	6
ATOM	546	CG	ASN	A	67	43.712	21.118	39.578	1.00	38.78	6
ATOM	547	OD1	ASN	A	67	44.674	21.841	39.878	1.00	43.34	8
ATOM	548	ND2	ASN	A	67	43.626	19.845	39.956	1.00	37.14	7
ATOM	549	C	ASN	A	67	41.020	23.554	38.314	1.00	28.41	6
ATOM	550	O	ASN	A	67	41.494	24.354	37.499	1.00	28.05	8
ATOM	551	N	THR	A	68	39.733	23.221	38.361	1.00	25.32	7
ATOM	552	CA	THR	A	68	38.767	23.791	37.416	1.00	21.75	6
ATOM	553	CB	THR	A	68	37.438	23.111	37.500	1.00	16.99	6
ATOM	554	OG1	THR	A	68	37.620	21.695	37.371	1.00	16.99	8
ATOM	555	CG2	THR	A	68	36.549	23.591	36.359	1.00	17.59	6
ATOM	556	C	THR	A	68	38.633	25.263	37.732	1.00	22.13	6
ATOM	557	O	THR	A	68	38.529	26.088	36.830	1.00	21.97	8
ATOM	558	N	LEU	A	69	38.645	25.582	39.023	1.00	22.32	7
ATOM	559	CA	LEU	A	69	38.535	26.956	39.482	1.00	23.97	6
ATOM	560	CB	LEU	A	69	38.376	26.982	41.000	1.00	24.99	6
ATOM	561	CG	LEU	A	69	37.023	26.527	41.548	1.00	29.08	6
ATOM	562	CD1	LEU	A	69	37.087	26.416	43.066	1.00	30.99	6
ATOM	563	CD2	LEU	A	69	35.942	27.528	41.120	1.00	28.69	6
ATOM	564	C	LEU	A	69	39.772	27.757	39.088	1.00	24.90	6
ATOM	565	O	LEU	A	69	39.683	28.921	38.674	1.00	25.04	8
ATOM	566	N	MET	A	70	40.932	27.128	39.218	1.00	24.67	7
ATOM	567	CA	MET	A	70	42.183	27.794	38.897	1.00	23.62	6
ATOM	568	CB	MET	A	70	43.358	26.953	39.380	1.00	26.92	6
ATOM	569	CG	MET	A	70	43.418	26.751	40.884	1.00	26.69	6
ATOM	570	SD	MET	A	70	44.970	25.929	41.325	1.00	30.71	16
ATOM	571	CE	MET	A	70	46.137	27.077	40.642	1.00	23.20	6
ATOM	572	C	MET	A	70	42.324	28.040	37.412	1.00	21.62	6
ATOM	573	O	MET	A	70	42.903	29.041	36.982	1.00	18.99	8
ATOM	574	N	GLU	A	71	41.769	27.122	36.632	1.00	23.93	7
ATOM	575	CA	GLU	A	71	41.859	27.204	35.189	1.00	24.41	6
ATOM	576	CB	GLU	A	71	41.681	25.814	34.582	1.00	26.22	6
ATOM	577	CG	GLU	A	71	42.224	25.695	33.167	1.00	31.75	6
ATOM	578	CD	GLU	A	71	43.737	25.905	33.099	1.00	33.00	6
ATOM	579	OE1	GLU	A	71	44.288	25.855	31.983	1.00	35.84	8
ATOM	580	OE2	GLU	A	71	44.377	26.116	34.154	1.00	30.13	8
ATOM	581	C	GLU	A	71	40.845	28.160	34.592	1.00	21.86	6
ATOM	582	O	GLU	A	71	41.144	28.851	33.626	1.00	21.54	8
ATOM	583	N	ALA	A	72	39.649	28.197	35.169	1.00	19.22	7
ATOM	584	CA	ALA	A	72	38.589	29.067	34.684	1.00	19.39	6
ATOM	585	CB	ALA	A	72	37.298	28.743	35.397	1.00	19.23	6
ATOM	586	C	ALA	A	72	38.931	30.536	34.899	1.00	26.72	6
ATOM	587	O	ALA	A	72	38.711	31.383	34.016	1.00	26.12	8
ATOM	588	N	GLU	A	73	39.470	30.835	36.079	1.00	28.44	7
ATOM	589	CA	GLU	A	73	39.820	32.202	36.436	1.00	29.44	6
ATOM	590	CB	GLU	A	73	40.157	32.282	37.931	1.00	25.84	6
ATOM	591	CG	GLU	A	73	40.646	33.655	38.349	1.00	27.51	6
ATOM	592	CD	GLU	A	73	40.840	33.806	39.841	1.00	29.38	6
ATOM	593	OE1	GLU	A	73	39.841	33.776	40.582	1.00	32.49	8
ATOM	594	OE2	GLU	A	73	41.996	33.960	40.277	1.00	31.77	8

77/263

Figure 17-10

ATOM	595	C	GLU	A	73	40.946	32.840	35.615	1.00	31.83	6
ATOM	596	O	GLU	A	73	40.859	34.024	35.259	1.00	33.52	8
ATOM	597	N	ARG	A	74	41.992	32.071	35.309	1.00	31.45	7
ATOM	598	CA	ARG	A	74	43.128	32.611	34.557	1.00	30.65	6
ATOM	599	CB	ARG	A	74	44.405	31.826	34.874	1.00	32.12	6
ATOM	600	CG	ARG	A	74	44.514	30.467	34.205	1.00	31.42	6
ATOM	601	CD	ARG	A	74	45.702	29.714	34.754	1.00	30.73	6
ATOM	602	NE	ARG	A	74	46.041	28.561	33.933	1.00	34.18	7
ATOM	603	CZ	ARG	A	74	46.646	28.634	32.748	1.00	35.55	6
ATOM	604	NH1	ARG	A	74	46.989	29.818	32.232	1.00	29.64	7
ATOM	605	NH2	ARG	A	74	46.906	27.514	32.079	1.00	34.07	7
ATOM	606	C	ARG	A	74	42.894	32.623	33.051	1.00	28.61	6
ATOM	607	O	ARG	A	74	43.431	33.465	32.338	1.00	24.38	8
ATOM	608	N	CYS	A	75	42.107	31.673	32.566	1.00	28.32	7
ATOM	609	CA	CYS	A	75	41.796	31.619	31.148	1.00	32.42	6
ATOM	610	CB	CYS	A	75	41.687	30.167	30.682	1.00	32.91	6
ATOM	611	SG	CYS	A	75	43.281	29.296	30.777	1.00	37.09	16
ATOM	612	C	CYS	A	75	40.489	32.382	30.956	1.00	33.10	6
ATOM	613	O	CYS	A	75	40.029	32.598	29.834	1.00	30.74	8
ATOM	614	N	GLN	A	76	39.914	32.787	32.088	1.00	34.42	7
ATOM	615	CA	GLN	A	76	38.691	33.575	32.144	1.00	33.20	6
ATOM	616	CB	GLN	A	76	38.986	34.962	31.578	1.00	32.09	6
ATOM	617	CG	GLN	A	76	38.089	36.064	32.094	1.00	39.46	6
ATOM	618	CD	GLN	A	76	38.479	36.541	33.480	1.00	41.47	6
ATOM	619	OE1	GLN	A	76	38.574	35.755	34.426	1.00	45.02	8
ATOM	620	NE2	GLN	A	76	38.703	37.846	33.606	1.00	42.22	7
ATOM	621	C	GLN	A	76	37.561	32.920	31.358	1.00	33.20	6
ATOM	622	O	GLN	A	76	36.732	33.598	30.760	1.00	34.19	8
ATOM	623	N	CYS	A	77	37.522	31.598	31.370	1.00	31.81	7
ATOM	624	CA	CYS	A	77	36.511	30.862	30.627	1.00	31.47	6
ATOM	625	CB	CYS	A	77	37.187	30.181	29.454	1.00	30.25	6
ATOM	626	SG	CYS	A	77	38.479	29.071	30.044	1.00	33.94	16
ATOM	627	C	CYS	A	77	35.851	29.795	31.498	1.00	31.97	6
ATOM	628	O	CYS	A	77	36.335	29.503	32.590	1.00	35.15	8
ATOM	629	N	VAL	A	78	34.750	29.216	31.018	1.00	30.78	7
ATOM	630	CA	VAL	A	78	34.069	28.139	31.747	1.00	30.55	6
ATOM	631	CB	VAL	A	78	32.539	28.287	31.720	1.00	30.06	6
ATOM	632	CG1	VAL	A	78	31.881	27.030	32.293	1.00	28.23	6
ATOM	633	CG2	VAL	A	78	32.129	29.503	32.526	1.00	30.67	6
ATOM	634	C	VAL	A	78	34.420	26.794	31.110	1.00	29.80	6
ATOM	635	O	VAL	A	78	33.851	26.422	30.077	1.00	29.65	8
ATOM	636	N	PRO	A	79	35.337	26.033	31.739	1.00	28.55	7
ATOM	637	CD	PRO	A	79	35.985	26.335	33.025	1.00	24.39	6
ATOM	638	CA	PRO	A	79	35.793	24.724	31.261	1.00	28.89	6
ATOM	639	CB	PRO	A	79	36.622	24.218	32.434	1.00	24.49	6
ATOM	640	CG	PRO	A	79	37.239	25.500	32.922	1.00	25.68	6
ATOM	641	C	PRO	A	79	34.668	23.776	30.881	1.00	30.13	6
ATOM	642	O	PRO	A	79	33.697	23.624	31.615	1.00	30.87	8
ATOM	643	N	LYS	A	80	34.796	23.136	29.727	1.00	33.44	7
ATOM	644	CA	LYS	A	80	33.758	22.216	29.303	1.00	38.52	6
ATOM	645	CB	LYS	A	80	34.202	21.421	28.076	1.00	45.18	6
ATOM	646	CG	LYS	A	80	35.450	20.589	28.278	1.00	55.18	6
ATOM	647	CD	LYS	A	80	35.788	19.827	27.000	1.00	60.80	6
ATOM	648	CE	LYS	A	80	37.035	18.976	27.168	1.00	64.25	6
ATOM	649	NZ	LYS	A	80	37.367	18.252	25.911	1.00	68.95	7
ATOM	650	C	LYS	A	80	33.411	21.267	30.443	1.00	36.56	6
ATOM	651	O	LYS	A	80	34.293	20.775	31.164	1.00	31.61	8
ATOM	652	N	GLY	A	81	32.112	21.035	30.602	1.00	32.57	7
ATOM	653	CA	GLY	A	81	31.634	20.155	31.648	1.00	29.81	6
ATOM	654	C	GLY	A	81	31.477	20.884	32.965	1.00	28.30	6
ATOM	655	O	GLY	A	81	30.544	20.612	33.723	1.00	25.49	8
ATOM	656	N	ALA	A	82	32.380	21.830	33.218	1.00	25.99	7
ATOM	657	CA	ALA	A	82	32.384	22.602	34.458	1.00	26.72	6
ATOM	658	CB	ALA	A	82	33.485	23.674	34.406	1.00	22.64	6
ATOM	659	C	ALA	A	82	31.066	23.245	34.886	1.00	27.84	6
ATOM	660	O	ALA	A	82	30.729	23.224	36.068	1.00	30.00	8

78/263 Figure 17-11

ATOM	661	N	ARG	A	83	30.310	23.811	33.951	1.00	31.15	7
ATOM	662	CA	ARG	A	83	29.071	24.462	34.345	1.00	32.50	6
ATOM	663	CB	ARG	A	83	28.285	24.941	33.127	1.00	37.19	6
ATOM	664	CG	ARG	A	83	27.439	26.189	33.408	1.00	42.23	6
ATOM	665	CD	ARG	A	83	26.480	26.020	34.585	1.00	48.02	6
ATOM	666	NE	ARG	A	83	25.904	27.303	34.996	1.00	53.00	7
ATOM	667	CZ	ARG	A	83	25.046	27.460	36.005	1.00	56.84	6
ATOM	668	NH1	ARG	A	83	24.649	26.413	36.724	1.00	53.05	7
ATOM	669	NH2	ARG	A	83	24.588	28.672	36.304	1.00	58.03	7
ATOM	670	C	ARG	A	83	28.208	23.531	25.189	1.00	31.50	6
ATOM	671	O	ARG	A	83	28.056	23.749	36.386	1.00	29.62	8
ATOM	672	N	GLU	A	84	27.648	22.491	34.581	1.00	33.06	7
ATOM	673	CA	GLU	A	84	26.819	21.568	35.343	1.00	35.40	6
ATOM	674	CB	GLU	A	84	26.112	20.562	34.417	1.00	37.35	6
ATOM	675	CG	GLU	A	84	26.989	19.684	33.496	1.00	40.01	6
ATOM	676	CD	GLU	A	84	27.551	20.418	32.267	1.00	44.49	6
ATOM	677	OE1	GLU	A	84	27.925	19.723	31.292	1.00	41.12	8
ATOM	678	OE2	GLU	A	84	27.636	21.671	32.270	1.00	41.01	8
ATOM	679	C	GLU	A	84	27.617	20.823	36.417	1.00	35.42	6
ATOM	680	O	GLU	A	84	27.246	20.816	37.594	1.00	34.66	8
ATOM	681	N	LYS	A	85	28.727	20.226	36.002	1.00	35.21	7
ATOM	682	CA	LYS	A	85	29.604	19.450	36.878	1.00	37.93	6
ATOM	683	CB	LYS	A	85	30.841	19.030	36.076	1.00	40.61	6
ATOM	684	CG	LYS	A	85	31.739	17.977	36.706	1.00	42.63	6
ATOM	685	CD	LYS	A	85	31.038	16.640	36.872	1.00	45.48	6
ATOM	686	CE	LYS	A	85	32.054	15.523	37.078	1.00	45.60	6
ATOM	687	NZ	LYS	A	85	33.032	15.833	38.154	1.00	46.16	7
ATOM	688	C	LYS	A	85	30.032	20.159	38.175	1.00	37.56	6
ATOM	689	O	LYS	A	85	30.161	19.516	39.222	1.00	38.40	8
ATOM	690	N	TYR	A	86	30.254	21.472	38.116	1.00	35.60	7
ATOM	691	CA	TYR	A	86	30.671	22.216	39.307	1.00	32.67	6
ATOM	692	CB	TYR	A	86	32.151	22.610	39.200	1.00	32.09	6
ATOM	693	CG	TYR	A	86	33.065	21.424	38.995	1.00	33.63	6
ATOM	694	CD1	TYR	A	86	33.120	20.393	39.932	1.00	32.12	6
ATOM	695	CE1	TYR	A	86	33.918	19.266	39.723	1.00	33.59	6
ATOM	696	CD2	TYR	A	86	33.839	21.306	37.841	1.00	33.82	6
ATOM	697	CE2	TYR	A	86	34.645	20.178	37.623	1.00	34.55	6
ATOM	698	CZ	TYR	A	86	34.675	19.162	38.566	1.00	32.38	6
ATOM	699	OH	TYR	A	86	35.431	18.034	38.336	1.00	29.17	8
ATOM	700	C	TYR	A	86	29.831	23.455	39.597	1.00	30.21	6
ATOM	701	O	TYR	A	86	30.192	24.265	40.445	1.00	29.12	8
ATOM	702	N	ASN	A	87	28.712	23.594	38.893	1.00	29.44	7
ATOM	703	CA	ASN	A	87	27.797	24.717	39.086	1.00	28.58	6
ATOM	704	CB	ASN	A	87	27.154	24.618	40.470	1.00	25.63	6
ATOM	705	CG	ASN	A	87	25.871	25.428	40.596	1.00	28.05	6
ATOM	706	OD1	ASN	A	87	25.275	25.477	41.672	1.00	31.32	8
ATOM	707	ND2	ASN	A	87	25.434	26.055	39.506	1.00	38.35	7
ATOM	708	C	ASN	A	87	28.580	26.015	38.963	1.00	30.35	6
ATOM	709	O	ASN	A	87	28.319	26.981	39.677	1.00	32.07	8
ATOM	710	N	ILE	A	88	29.545	26.019	38.051	1.00	32.05	7
ATOM	711	CA	ILE	A	88	30.407	27.173	37.809	1.00	33.77	6
ATOM	712	CB	ILE	A	88	31.894	26.734	37.776	1.00	36.13	6
ATOM	713	CG2	ILE	A	88	32.759	27.831	37.201	1.00	37.80	6
ATOM	714	CG1	ILE	A	88	32.357	26.342	39.178	1.00	38.92	6
ATOM	715	CD1	ILE	A	88	32.350	27.483	40.176	1.00	41.44	6
ATOM	716	C	ILE	A	88	30.085	27.857	36.482	1.00	32.28	6
ATOM	717	O	ILE	A	88	29.708	27.196	35.520	1.00	32.72	8
ATOM	718	N	GLY	A	89	30.237	29.179	36.438	1.00	31.56	7
ATOM	719	CA	GLY	A	89	29.994	29.915	35.207	1.00	30.84	6
ATOM	720	C	GLY	A	89	28.696	30.689	35.093	1.00	32.17	6
ATOM	721	O	GLY	A	89	28.628	31.670	34.349	1.00	30.42	8
ATOM	722	N	GLY	A	90	27.670	30.257	35.821	1.00	31.51	7
ATOM	723	CA	GLY	A	90	26.387	30.937	35.756	1.00	32.92	6
ATOM	724	C	GLY	A	90	26.316	32.246	36.524	1.00	34.32	6
ATOM	725	O	GLY	A	90	27.302	32.671	37.129	1.00	33.97	8
ATOM	726	N	TYR	A	91	25.144	32.882	36.504	1.00	33.88	7

79/263
Figure 17-12

ATOM	727	CA	TYR	A	91	24.924	34.146	37.206	1.00	35.76	6
ATOM	728	CB	TYR	A	91	23.465	34.589	37.058	1.00	38.10	6
ATOM	729	CG	TYR	A	91	23.089	35.733	37.990	1.00	42.40	6
ATOM	730	CD1	TYR	A	91	23.417	37.057	37.688	1.00	43.57	6
ATOM	731	CE1	TYR	A	91	23.105	38.106	38.577	1.00	42.44	6
ATOM	732	CD2	TYR	A	91	22.444	35.484	39.205	1.00	44.07	6
ATOM	733	CE2	TYR	A	91	22.132	36.526	40.097	1.00	42.67	6
ATOM	734	CZ	TYR	A	91	22.462	37.825	39.775	1.00	42.41	6
ATOM	735	OH	TYR	A	91	22.130	38.835	40.646	1.00	43.69	8
ATOM	736	C	TYR	A	91	25.242	34.082	38.701	1.00	34.15	6
ATOM	737	O	TYR	A	91	25.821	35.014	39.266	1.00	29.52	8
ATOM	738	N	GLU	A	92	24.837	32.986	39.333	1.00	34.78	7
ATOM	739	CA	GLU	A	92	25.024	32.797	40.767	1.00	38.46	6
ATOM	740	CB	GLU	A	92	24.233	31.564	41.211	1.00	43.99	6
ATOM	741	CG	GLU	A	92	23.932	31.489	42.700	1.00	52.10	6
ATOM	742	CD	GLU	A	92	23.294	30.161	43.097	1.00	58.00	6
ATOM	743	OE1	GLU	A	92	24.001	29.126	43.058	1.00	60.63	8
ATOM	744	OE2	GLU	A	92	22.087	30.149	43.434	1.00	59.58	8
ATOM	745	C	GLU	A	92	26.492	32.669	41.208	1.00	36.42	6
ATOM	746	O	GLU	A	92	26.902	33.287	42.193	1.00	32.92	8
ATOM	747	N	ASN	A	93	27.280	31.883	40.473	1.00	34.12	7
ATOM	748	CA	ASN	A	93	28.693	31.671	40.808	1.00	33.24	6
ATOM	749	CB	ASN	A	93	28.871	30.259	41.364	1.00	28.52	6
ATOM	750	CG	ASN	A	93	27.734	29.859	42.299	1.00	27.45	6
ATOM	751	OD1	ASN	A	93	27.547	30.457	43.355	1.00	21.76	8
ATOM	752	ND2	ASN	A	93	26.956	28.853	41.895	1.00	21.79	7
ATOM	753	C	ASN	A	93	29.529	31.843	39.535	1.00	35.04	6
ATOM	754	O	ASN	A	93	30.160	30.898	39.059	1.00	33.81	8
ATOM	755	N	PRO	A	94	29.583	33.081	39.010	1.00	36.19	7
ATOM	756	CD	PRO	A	94	28.970	34.231	39.690	1.00	34.62	6
ATOM	757	CA	PRO	A	94	30.274	33.560	37.808	1.00	34.80	6
ATOM	758	CB	PRO	A	94	29.924	35.050	37.791	1.00	33.94	6
ATOM	759	CG	PRO	A	94	28.619	35.095	38.516	1.00	36.13	6
ATOM	760	C	PRO	A	94	31.775	33.379	37.733	1.00	34.63	6
ATOM	761	O	PRO	A	94	32.443	33.103	38.730	1.00	34.72	8
ATOM	762	N	VAL	A	95	32.299	33.556	36.526	1.00	33.57	7
ATOM	763	CA	VAL	A	95	33.735	33.499	36.307	1.00	30.31	6
ATOM	764	CB	VAL	A	95	34.085	33.171	34.841	1.00	29.88	6
ATOM	765	CG1	VAL	A	95	35.561	33.453	34.574	1.00	29.53	6
ATOM	766	CG2	VAL	A	95	33.795	31.713	34.563	1.00	28.05	6
ATOM	767	C	VAL	A	95	34.195	34.910	36.624	1.00	29.86	6
ATOM	768	O	VAL	A	95	33.524	35.879	36.272	1.00	29.07	8
ATOM	769	N	SER	A	96	35.318	35.019	37.317	1.00	30.89	7
ATOM	770	CA	SER	A	96	35.889	36.310	37.687	1.00	32.27	6
ATOM	771	CB	SER	A	96	34.885	37.145	38.501	1.00	30.16	6
ATOM	772	OG	SER	A	96	34.600	36.545	39.756	1.00	26.77	8
ATOM	773	C	SER	A	96	37.111	35.993	38.537	1.00	32.96	6
ATOM	774	O	SER	A	96	37.603	34.865	38.511	1.00	33.77	8
ATOM	775	N	TYR	A	97	37.609	36.973	39.282	1.00	32.66	7
ATOM	776	CA	TYR	A	97	38.753	36.712	40.132	1.00	31.95	6
ATOM	777	CB	TYR	A	97	39.838	37.766	39.923	1.00	31.81	6
ATOM	778	CG	TYR	A	97	40.416	37.729	38.525	1.00	30.39	6
ATOM	779	CD1	TYR	A	97	39.820	38.434	37.479	1.00	30.63	6
ATOM	780	CE1	TYR	A	97	40.327	38.358	36.178	1.00	28.49	6
ATOM	781	CD2	TYR	A	97	41.536	36.945	38.236	1.00	28.43	6
ATOM	782	CE2	TYR	A	97	42.046	36.858	36.942	1.00	24.73	6
ATOM	783	CZ	TYR	A	97	41.437	37.565	35.919	1.00	27.27	6
ATOM	784	OH	TYR	A	97	41.915	37.455	34.633	1.00	26.70	8
ATOM	785	C	TYR	A	97	38.350	36.618	41.596	1.00	31.10	6
ATOM	786	O	TYR	A	97	39.178	36.735	42.495	1.00	33.01	8
ATOM	787	N	ALA	A	98	37.059	36.398	41.818	1.00	31.11	7
ATOM	788	CA	ALA	A	98	36.510	36.241	43.160	1.00	30.06	6
ATOM	789	CB	ALA	A	98	35.141	36.920	43.256	1.00	27.71	6
ATOM	790	C	ALA	A	98	36.350	34.736	43.357	1.00	31.24	6
ATOM	791	O	ALA	A	98	36.335	34.238	44.487	1.00	29.66	8
ATOM	792	N	MET	A	99	36.249	34.030	42.230	1.00	29.50	7

80/263

Figure 17-13

ATOM	793	CA	MET	A	99	36.048	32.589	42.207	1.00	29.89	6
ATOM	794	CB	MET	A	99	35.774	32.123	40.778	1.00	30.48	6
ATOM	795	CG	MET	A	99	36.942	32.265	39.822	1.00	29.63	6
ATOM	796	SD	MET	A	99	36.426	31.939	38.126	1.00	29.78	16
ATOM	797	CE	MET	A	99	35.629	30.273	38.347	1.00	25.05	6
ATOM	798	C	MET	A	99	37.199	31.800	42.783	1.00	30.81	6
ATOM	799	O	MET	A	99	36.993	30.757	43.406	1.00	30.59	8
ATOM	800	N	PHE	A	100	38.417	32.274	42.569	1.00	32.09	7
ATOM	801	CA	PHE	A	100	39.554	31.557	43.114	1.00	33.87	6
ATOM	802	CB	PHE	A	100	40.322	30.817	42.029	1.00	33.95	6
ATOM	803	CG	PHE	A	100	41.434	29.979	42.578	1.00	41.14	6
ATOM	804	CD1	PHE	A	100	41.152	28.862	43.364	1.00	41.84	6
ATOM	805	CD2	PHE	A	100	42.768	30.339	42.372	1.00	42.18	6
ATOM	806	CE1	PHE	A	100	42.185	28.115	43.941	1.00	41.63	6
ATOM	807	CE2	PHE	A	100	43.808	29.600	42.944	1.00	40.50	6
ATOM	808	CZ	PHE	A	100	43.517	28.487	43.729	1.00	39.89	6
ATOM	809	C	PHE	A	100	40.519	32.438	43.895	1.00	33.98	6
ATOM	810	O	PHE	A	100	40.706	32.231	45.088	1.00	38.21	8
ATOM	811	N	THR	A	101	41.137	33.415	43.245	1.00	28.09	7
ATOM	812	CA	THR	A	101	42.063	34.261	43.969	1.00	22.19	6
ATOM	813	CB	THR	A	101	42.623	35.378	43.072	1.00	22.48	6
ATOM	814	OG1	THR	A	101	43.441	34.795	42.052	1.00	21.99	8
ATOM	815	CG2	THR	A	101	43.468	36.335	43.876	1.00	15.00	6
ATOM	816	C	THR	A	101	41.408	34.860	45.205	1.00	21.71	6
ATOM	817	C	THR	A	101	41.988	34.845	46.282	1.00	23.82	8
ATOM	818	N	GLY	A	102	40.197	35.377	45.068	1.00	21.79	7
ATOM	819	CA	GLY	A	102	39.533	35.947	46.231	1.00	21.23	6
ATOM	820	C	GLY	A	102	39.072	34.833	47.153	1.00	23.03	6
ATOM	821	O	GLY	A	102	39.209	34.909	48.378	1.00	20.41	8
ATOM	822	N	SER	A	103	38.512	33.792	46.544	1.00	22.59	7
ATOM	823	CA	SER	A	103	38.028	32.640	47.276	1.00	26.51	6
ATOM	824	CB	SER	A	103	37.454	31.598	46.314	1.00	28.10	6
ATOM	825	OG	SER	A	103	36.314	32.099	45.639	1.00	32.01	8
ATOM	826	C	SER	A	103	39.188	32.040	48.032	1.00	27.73	6
ATOM	827	O	SER	A	103	39.019	31.544	49.144	1.00	30.61	8
ATOM	828	N	SER	A	104	40.364	32.080	47.410	1.00	28.76	7
ATOM	829	CA	SER	A	104	41.590	31.552	48.008	1.00	28.55	6
ATOM	830	CB	SER	A	104	42.769	31.683	47.039	1.00	28.74	6
ATOM	831	OG	SER	A	104	42.501	31.044	45.804	1.00	35.04	8
ATOM	832	C	SER	A	104	41.870	32.401	49.226	1.00	25.67	6
ATOM	833	O	SER	A	104	42.026	31.897	50.338	1.00	25.17	8
ATOM	834	N	LEU	A	105	41.909	33.705	48.986	1.00	23.91	7
ATOM	835	CA	LEU	A	105	42.163	34.698	50.008	1.00	23.01	6
ATOM	836	CB	LEU	A	105	42.049	36.082	49.382	1.00	23.57	6
ATOM	837	CG	LEU	A	105	43.158	37.091	49.672	1.00	26.30	6
ATOM	838	CD1	LEU	A	105	44.502	36.551	49.178	1.00	22.38	6
ATOM	839	CD2	LEU	A	105	42.823	38.413	48.984	1.00	27.36	6
ATOM	840	C	LEU	A	105	41.187	34.559	51.182	1.00	23.48	6
ATOM	841	O	LEU	A	105	41.604	34.448	52.331	1.00	21.60	8
ATOM	842	N	ALA	A	106	39.887	34.556	50.897	1.00	25.32	7
ATOM	843	CA	ALA	A	106	38.884	34.423	51.957	1.00	26.04	6
ATOM	844	CB	ALA	A	106	37.471	34.423	51.358	1.00	24.28	6
ATOM	845	C	ALA	A	106	39.088	33.158	52.790	1.00	25.76	6
ATOM	846	O	ALA	A	106	38.953	33.186	54.015	1.00	22.75	8
ATOM	847	N	THR	A	107	39.410	32.057	52.111	1.00	25.65	7
ATOM	848	CA	THR	A	107	39.620	30.760	52.754	1.00	25.54	6
ATOM	849	CB	THR	A	107	39.706	29.637	51.713	1.00	21.92	6
ATOM	850	OG1	THR	A	107	38.559	29.688	50.868	1.00	26.40	8
ATOM	851	CG2	THR	A	107	39.742	28.295	52.387	1.00	17.36	6
ATOM	852	C	THR	A	107	40.901	30.720	53.583	1.00	28.16	6
ATOM	853	O	THR	A	107	40.906	30.254	54.727	1.00	28.07	8
ATOM	854	N	GLY	A	108	41.994	31.191	52.996	1.00	28.51	7
ATOM	855	CA	GLY	A	108	43.247	31.187	53.718	1.00	28.37	6
ATOM	856	C	GLY	A	108	43.027	31.921	55.019	1.00	30.26	6
ATOM	857	O	GLY	A	108	43.502	31.499	56.076	1.00	32.98	8
ATOM	858	N	SER	A	109	42.283	33.018	54.942	1.00	24.81	7

Figure 17-14

ATOM	859	CA	SER	A	109	42.002	33.810	56.119	1.00	24.86	6
ATOM	860	CB	SER	A	109	41.222	35.066	55.727	1.00	24.74	6
ATOM	861	OG	SER	A	109	41.992	35.898	54.872	1.00	21.07	8
ATOM	862	C	SER	A	109	41.240	32.996	57.173	1.00	27.89	6
ATOM	863	O	SER	A	109	41.424	33.214	58.377	1.00	30.92	8
ATOM	864	N	THR	A	110	40.389	32.064	56.744	1.00	23.91	7
ATOM	865	CA	THR	A	110	39.676	31.259	57.721	1.00	24.80	6
ATOM	866	CB	THR	A	110	38.641	30.290	57.074	1.00	29.65	6
ATOM	867	OG1	THR	A	110	37.469	31.016	56.669	1.00	30.45	8
ATOM	868	CG2	THR	A	110	38.228	29.205	58.067	1.00	29.00	6
ATOM	869	C	THR	A	110	40.712	30.449	58.478	1.00	24.34	6
ATOM	870	O	THR	A	110	40.615	30.282	59.699	1.00	24.74	8
ATOM	871	N	VAL	A	111	41.715	29.954	57.764	1.00	23.01	7
ATOM	872	CA	VAL	A	111	42.759	29.173	58.416	1.00	24.13	6
ATOM	873	CB	VAL	A	111	43.695	28.495	57.391	1.00	25.77	6
ATOM	874	CG1	VAL	A	111	44.845	27.773	58.121	1.00	22.51	6
ATOM	875	CG2	VAL	A	111	42.888	27.502	56.534	1.00	22.67	6
ATOM	876	C	VAL	A	111	43.576	30.071	59.329	1.00	23.14	6
ATOM	877	O	VAL	A	111	43.720	29.793	60.518	1.00	24.11	8
ATOM	878	N	GLN	A	112	44.101	31.156	58.772	1.00	24.94	7
ATOM	879	CA	GLN	A	112	44.895	32.100	59.554	1.00	25.12	6
ATOM	880	CB	GLN	A	112	45.082	33.413	58.779	1.00	25.14	6
ATOM	881	CG	GLN	A	112	45.545	33.224	57.330	1.00	28.51	6
ATOM	882	CD	GLN	A	112	45.789	34.534	56.594	1.00	29.13	6
ATOM	883	OE1	GLN	A	112	46.779	35.219	56.837	1.00	31.22	8
ATOM	884	NE2	GLN	A	112	44.877	34.890	55.694	1.00	29.31	7
ATOM	885	C	GLN	A	112	44.107	32.362	60.827	1.00	24.62	6
ATOM	886	O	GLN	A	112	44.647	32.311	61.939	1.00	21.10	8
ATOM	887	N	ALA	A	113	42.813	32.622	60.644	1.00	24.41	7
ATOM	888	CA	ALA	A	113	41.914	32.904	61.751	1.00	23.33	6
ATOM	889	CB	ALA	A	113	40.516	33.183	61.224	1.00	19.80	6
ATOM	890	C	ALA	A	113	41.901	31.733	62.729	1.00	25.34	6
ATOM	891	O	ALA	A	113	41.925	31.930	63.946	1.00	27.52	8
ATOM	892	N	ILE	A	114	41.859	30.509	62.211	1.00	24.39	7
ATOM	893	CA	ILE	A	114	41.867	29.356	63.106	1.00	24.49	6
ATOM	894	CB	ILE	A	114	41.524	28.042	62.371	1.00	23.46	6
ATOM	895	CG2	ILE	A	114	41.902	26.855	63.227	1.00	18.97	6
ATOM	896	CG1	ILE	A	114	40.030	28.015	62.034	1.00	21.17	6
ATOM	897	CD1	ILE	A	114	39.598	26.791	61.239	1.00	22.51	6
ATOM	898	C	ILE	A	114	43.230	29.227	63.757	1.00	24.32	6
ATOM	899	O	ILE	A	114	43.328	28.817	64.907	1.00	24.74	8
ATOM	900	N	GLU	A	115	44.280	29.580	63.019	1.00	26.58	7
ATOM	901	CA	GLU	A	115	45.638	29.518	63.551	1.00	25.89	6
ATOM	902	CB	GLU	A	115	46.639	29.992	62.508	1.00	22.63	6
ATOM	903	CG	GLU	A	115	46.554	29.264	61.192	1.00	20.39	6
ATOM	904	CD	GLU	A	115	17.668	29.670	60.244	1.00	21.39	6
ATOM	905	OE1	GLU	A	115	47.848	30.887	60.016	1.00	19.60	8
ATOM	906	OE2	GLU	A	115	18.362	28.769	59.722	1.00	22.53	8
ATOM	907	C	GLU	A	115	45.724	30.422	64.774	1.00	27.56	6
ATOM	908	O	GLU	A	115	46.173	30.006	65.837	1.00	25.98	8
ATOM	909	N	GLU	A	116	45.267	31.660	64.615	1.00	31.19	7
ATOM	910	CA	GLU	A	116	45.282	32.631	65.705	1.00	35.80	6
ATOM	911	CB	GLU	A	116	44.676	33.959	65.237	1.00	36.91	6
ATOM	912	CG	GLU	A	116	45.434	34.605	64.069	1.00	41.14	6
ATOM	913	CD	GLU	A	116	46.872	34.982	64.420	1.00	43.09	6
ATOM	914	OE1	GLU	A	116	47.072	35.886	65.267	1.00	43.42	8
ATOM	915	OE2	GLU	A	116	47.802	34.369	63.849	1.00	41.76	8
ATOM	916	C	GLU	A	116	44.543	32.131	66.947	1.00	35.11	6
ATOM	917	O	GLU	A	116	45.054	32.228	68.061	1.00	37.26	8
ATOM	918	N	PHE	A	117	43.343	31.598	66.761	1.00	34.30	7
ATOM	919	CA	PHE	A	117	42.577	31.096	67.893	1.00	34.44	6
ATOM	920	CB	PHE	A	117	41.300	30.399	67.415	1.00	35.45	6
ATOM	921	CG	PHE	A	117	40.383	29.979	68.533	1.00	37.14	6
ATOM	922	CD1	PHE	A	117	39.705	30.930	69.290	1.00	35.80	6
ATOM	923	CD2	PHE	A	117	40.196	28.630	68.832	1.00	41.05	6
ATOM	924	CE1	PHE	A	117	38.853	30.549	70.323	1.00	38.08	6

Figure 17-15

ATOM	925	CE2	PHE	A	117	39.338	28.234	69.874	1.00	40.44	5
ATOM	926	CZ	PHE	A	117	38.668	29.198	70.617	1.00	38.64	6
ATOM	927	C	PHE	A	117	43.424	30.094	68.669	1.00	34.24	6
ATOM	928	O	PHE	A	117	43.490	30.136	69.898	1.00	33.54	8
ATOM	929	N	LEU	A	118	44.069	29.194	67.933	1.00	33.14	7
ATOM	930	CA	LEU	A	118	44.898	28.158	68.523	1.00	32.62	6
ATOM	931	CB	LEU	A	118	45.155	27.056	67.488	1.00	30.59	6
ATOM	932	CG	LEU	A	118	43.900	26.297	67.038	1.00	27.87	6
ATOM	933	CD1	LEU	A	118	44.244	25.232	65.996	1.00	20.81	6
ATOM	934	CD2	LEU	A	118	43.259	25.662	68.257	1.00	28.37	6
ATOM	935	C	LEU	A	118	46.216	28.696	69.084	1.00	34.37	6
ATOM	936	O	LEU	A	118	46.983	27.964	69.708	1.00	36.15	8
ATOM	937	N	LYS	A	119	46.481	29.974	68.843	1.00	34.75	7
ATOM	938	CA	LYS	A	119	47.679	30.609	69.365	1.00	34.34	6
ATOM	939	CB	LYS	A	119	48.143	31.739	68.448	1.00	33.52	6
ATOM	940	CG	LYS	A	119	48.614	31.270	67.100	1.00	37.98	6
ATOM	941	CD	LYS	A	119	49.111	32.430	66.263	1.00	43.40	6
ATOM	942	CE	LYS	A	119	49.691	31.928	64.949	1.00	46.52	6
ATOM	943	NZ	LYS	A	119	50.167	33.050	64.092	1.00	51.48	7
ATOM	944	C	LYS	A	119	47.273	31.191	70.705	1.00	34.85	6
ATOM	945	O	LYS	A	119	48.112	31.465	71.562	1.00	38.12	8
ATOM	946	N	GLY	A	120	45.967	31.372	70.869	1.00	34.15	7
ATOM	947	CA	GLY	A	120	45.431	31.927	72.094	1.00	36.25	6
ATOM	948	C	GLY	A	120	44.860	33.310	71.851	1.00	39.02	6
ATOM	949	O	GLY	A	120	44.640	34.072	72.796	1.00	40.23	8
ATOM	950	N	ASN	A	121	44.619	33.644	70.586	1.00	38.48	7
ATOM	951	CA	ASN	A	121	44.079	34.956	70.247	1.00	37.47	6
ATOM	952	CB	ASN	A	121	44.928	35.624	69.170	1.00	39.57	6
ATOM	953	CG	ASN	A	121	46.340	35.871	69.622	1.00	41.81	6
ATOM	954	OD1	ASN	A	121	47.078	34.938	69.926	1.00	47.67	8
ATOM	955	ND2	ASN	A	121	46.727	37.134	69.675	1.00	43.63	7
ATOM	956	C	ASN	A	121	42.637	34.893	69.772	1.00	36.59	6
ATOM	957	O	ASN	A	121	42.037	33.818	69.704	1.00	34.08	8
ATOM	958	N	VAL	A	122	42.092	36.061	69.446	1.00	33.53	7
ATOM	959	CA	VAL	A	122	40.720	36.166	68.976	1.00	34.77	6
ATOM	960	CB	VAL	A	122	39.861	37.064	69.898	1.00	38.20	6
ATOM	961	CG1	VAL	A	122	38.418	37.096	69.388	1.00	37.55	6
ATOM	962	CG2	VAL	A	122	39.918	36.553	71.342	1.00	37.77	6
ATOM	963	C	VAL	A	122	40.731	36.781	67.596	1.00	31.08	6
ATOM	964	O	VAL	A	122	40.991	37.967	67.441	1.00	34.19	8
ATOM	965	N	ALA	A	123	40.451	35.975	66.588	1.00	31.14	7
ATOM	966	CA	ALA	A	123	40.451	36.476	65.231	1.00	30.26	6
ATOM	967	CB	ALA	A	123	41.307	35.588	64.327	1.00	32.14	6
ATOM	968	C	ALA	A	123	39.038	36.533	64.716	1.00	28.26	6
ATOM	969	O	ALA	A	123	38.132	35.924	65.281	1.00	29.28	8
ATOM	970	N	PHE	A	124	38.875	37.276	63.631	1.00	28.70	7
ATOM	971	CA	PHE	A	124	37.601	37.475	62.976	1.00	28.38	6
ATOM	972	CB	PHE	A	124	36.920	38.713	63.563	1.00	29.16	6
ATOM	973	CG	PHE	A	124	35.645	39.099	62.874	1.00	31.20	6
ATOM	974	CD1	PHE	A	124	34.679	38.139	62.564	1.00	32.00	6
ATOM	975	CD2	PHE	A	124	35.378	40.435	62.579	1.00	29.53	6
ATOM	976	CE1	PHE	A	124	33.463	38.510	61.973	1.00	30.74	6
ATOM	977	CE2	PHE	A	124	34.165	40.813	61.988	1.00	27.45	6
ATOM	978	CZ	PHE	A	124	33.207	39.847	61.686	1.00	28.72	6
ATOM	979	C	PHE	A	124	37.880	37.671	61.496	1.00	30.19	6
ATOM	980	O	PHE	A	124	38.427	38.695	61.095	1.00	32.10	8
ATOM	981	N	ASN	A	125	37.545	36.663	60.696	1.00	32.16	7
ATOM	982	CA	ASN	A	125	37.731	36.728	59.251	1.00	30.10	6
ATOM	983	CB	ASN	A	125	38.247	35.393	58.712	1.00	32.02	6
ATOM	984	CG	ASN	A	125	38.281	35.360	57.195	1.00	33.79	6
ATOM	985	OD1	ASN	A	125	38.754	36.306	56.556	1.00	31.85	8
ATOM	986	ND2	ASN	A	125	37.790	34.268	56.609	1.00	30.51	7
ATOM	987	C	ASN	A	125	36.403	37.083	58.584	1.00	29.80	6
ATOM	988	O	ASN	A	125	35.626	36.206	58.179	1.00	27.24	8
ATOM	989	N	PRO	A	126	36.135	38.386	58.451	1.00	28.25	7
ATOM	990	CD	PRO	A	126	36.997	39.516	58.833	1.00	29.22	6

Figure 17-16

ATOM	991	CA	PRO A 126	34.909	38.891	57.844	1.00	27.92	6
ATOM	992	CB	PRO A 126	35.139	40.407	57.856	1.00	29.07	6
ATOM	993	CG	PRO A 126	36.649	40.520	57.775	1.00	26.54	6
ATOM	994	C	PRO A 126	34.651	38.339	56.448	1.00	27.54	6
ATOM	995	O	PRO A 126	33.532	38.402	55.949	1.00	28.66	8
ATOM	996	N	ALA A 127	35.687	37.795	55.820	1.00	26.99	7
ATOM	997	CA	ALA A 127	35.548	37.244	54.477	1.00	26.54	6
ATOM	998	CB	ALA A 127	36.822	37.505	53.684	1.00	22.43	6
ATOM	999	C	ALA A 127	35.225	35.744	54.480	1.00	27.38	6
ATOM	1000	O	ALA A 127	35.038	35.140	53.423	1.00	29.04	8
ATOM	1001	N	GLY A 128	35.166	35.142	55.663	1.00	26.97	7
ATOM	1002	CA	GLY A 128	34.874	33.724	55.737	1.00	25.65	6
ATOM	1003	C	GLY A 128	33.389	33.486	55.880	1.00	26.17	6
ATOM	1004	O	GLY A 128	32.600	34.428	55.804	1.00	27.39	8
ATOM	1005	N	GLY A 129	32.998	32.234	56.083	1.00	23.87	7
ATOM	1006	CA	GLY A 129	31.588	31.936	56.236	1.00	25.17	6
ATOM	1007	C	GLY A 129	30.847	31.674	54.937	1.00	25.88	6
ATOM	1008	O	GLY A 129	29.643	31.908	54.848	1.00	25.07	8
ATOM	1009	N	MET A 130	31.566	31.198	53.927	1.00	25.69	7
ATOM	1010	CA	MET A 130	30.981	30.872	52.622	1.00	26.48	6
ATOM	1011	CB	MET A 130	32.103	30.907	51.567	1.00	28.53	6
ATOM	1012	CG	MET A 130	32.795	32.288	51.467	1.00	26.54	6
ATOM	1013	SD	MET A 130	34.413	32.366	50.613	1.00	26.29	16
ATOM	1014	CE	MET A 130	34.080	31.512	49.062	1.00	25.85	6
ATOM	1015	C	MET A 130	30.355	29.463	52.768	1.00	24.47	6
ATOM	1016	O	MET A 130	30.761	28.502	52.113	1.00	17.67	8
ATOM	1017	N	HIS A 131	29.347	29.389	53.636	1.00	23.28	7
ATOM	1018	CA	HIS A 131	28.647	28.161	54.019	1.00	26.33	6
ATOM	1019	CB	HIS A 131	27.685	28.485	55.180	1.00	26.98	6
ATOM	1020	CG	HIS A 131	26.663	29.540	54.862	1.00	28.50	6
ATOM	1021	CD2	HIS A 131	26.225	30.030	53.677	1.00	28.65	6
ATOM	1022	ND1	HIS A 131	25.906	30.166	55.831	1.00	33.04	7
ATOM	1023	CE1	HIS A 131	25.051	30.995	55.259	1.00	27.75	6
ATOM	1024	NE2	HIS A 131	25.224	30.932	53.952	1.00	26.97	7
ATOM	1025	C	HIS A 131	27.917	27.284	53.017	1.00	28.44	6
ATOM	1026	O	HIS A 131	27.434	26.214	53.390	1.00	31.15	3
ATOM	1027	N	HIS A 132	27.861	27.694	51.756	1.00	30.64	7
ATOM	1028	CA	HIS A 132	27.111	26.938	50.746	1.00	28.71	6
ATOM	1029	CB	HIS A 132	26.321	27.941	49.890	1.00	27.21	6
ATOM	1030	CG	HIS A 132	25.408	28.819	50.693	1.00	28.83	6
ATOM	1031	CD2	HIS A 132	25.111	30.137	50.578	1.00	28.92	6
ATOM	1032	ND1	HIS A 132	24.686	28.360	51.773	1.00	31.80	7
ATOM	1033	CE1	HIS A 132	23.981	29.353	52.285	1.00	29.95	6
ATOM	1034	NE2	HIS A 132	24.222	30.443	51.579	1.00	28.21	7
ATOM	1035	C	HIS A 132	27.889	25.970	49.851	1.00	28.51	6
ATOM	1036	O	HIS A 132	27.399	24.375	49.533	1.00	23.44	8
ATOM	1037	N	ALA A 133	29.093	26.379	49.455	1.00	27.94	7
ATOM	1038	CA	ALA A 133	29.958	25.586	48.579	1.00	26.99	6
ATOM	1039	CB	ALA A 133	31.295	26.303	48.392	1.00	21.87	6
ATOM	1040	C	ALA A 133	30.199	24.164	49.078	1.00	26.69	6
ATOM	1041	O	ALA A 133	30.703	23.973	50.182	1.00	28.25	8
ATOM	1042	N	PHE A 134	29.850	23.174	48.255	1.00	26.73	7
ATOM	1043	CA	PHE A 134	30.046	21.773	48.615	1.00	25.04	6
ATOM	1044	CB	PHE A 134	29.070	20.855	47.875	1.00	19.20	6
ATOM	1045	CG	PHE A 134	27.629	21.199	48.100	1.00	15.75	6
ATOM	1046	CD1	PHE A 134	26.929	21.960	47.169	1.00	14.83	6
ATOM	1047	CD2	PHE A 134	26.985	20.814	49.273	1.00	14.03	6
ATOM	1048	CE1	PHE A 134	25.614	22.336	47.404	1.00	14.84	6
ATOM	1049	CE2	PHE A 134	25.670	21.184	49.519	1.00	12.07	6
ATOM	1050	CZ	PHE A 134	24.985	21.949	48.581	1.00	14.59	6
ATOM	1051	C	PHE A 134	31.460	21.510	48.319	1.00	29.48	6
ATOM	1052	O	PHE A 134	32.291	22.066	47.822	1.00	33.19	8
ATOM	1053	N	LYS A 135	31.713	20.045	48.620	1.00	31.52	7
ATOM	1054	CA	LYS A 135	33.012	19.427	48.427	1.00	29.15	6
ATOM	1055	CB	LYS A 135	32.923	17.971	48.885	1.00	29.45	6
ATOM	1056	CG	LYS A 135	34.152	17.131	48.638	1.00	32.46	6

84/263

Figure 17-17

ATOM	1057	CD	LYS	A	135	33.965	15.734	49.221	1.00	29.67	6
ATOM	1058	CE	LYS	A	135	34.234	15.703	50.716	1.00	30.09	6
ATOM	1059	NZ	LYS	A	135	35.679	15.973	51.001	1.00	26.25	7
ATOM	1060	C	LYS	A	135	33.513	19.516	46.993	1.00	30.22	6
ATOM	1061	O	LYS	A	135	34.714	19.672	46.763	1.00	30.00	8
ATOM	1062	N	SER	A	136	32.600	19.434	46.028	1.00	31.69	7
ATOM	1063	CA	SER	A	136	32.995	19.489	44.619	1.00	32.88	6
ATOM	1064	CB	SER	A	136	33.038	18.077	44.040	1.00	31.41	6
ATOM	1065	OG	SER	A	136	33.882	17.241	44.810	1.00	35.41	8
ATOM	1066	C	SER	A	136	32.097	20.347	43.727	1.00	33.55	6
ATOM	1067	O	SER	A	136	31.921	20.031	42.553	1.00	36.11	8
ATOM	1068	N	ARG	A	137	31.536	21.425	44.262	1.00	30.61	7
ATOM	1069	CA	ARG	A	137	30.564	22.272	43.459	1.00	32.28	6
ATOM	1070	CB	ARG	A	137	29.324	21.554	43.202	1.00	35.91	6
ATOM	1071	CG	ARG	A	137	28.224	22.458	42.627	1.00	43.90	6
ATOM	1072	CD	ARG	A	137	26.819	21.836	42.751	1.00	48.28	6
ATOM	1073	NE	ARG	A	137	26.571	20.767	41.787	1.00	53.38	7
ATOM	1074	CZ	ARG	A	137	26.150	20.960	40.538	1.00	55.30	6
ATOM	1075	NH1	ARG	A	137	25.921	22.185	40.090	1.00	54.06	7
ATOM	1076	NH2	ARG	A	137	25.969	19.922	39.728	1.00	58.96	7
ATOM	1077	C	ARG	A	137	30.405	23.631	44.113	1.00	30.24	6
ATOM	1078	O	ARG	A	137	30.380	23.748	45.338	1.00	23.11	8
ATOM	1079	N	ALA	A	138	30.219	24.653	43.279	1.00	27.33	7
ATOM	1080	CA	ALA	A	138	29.944	26.000	43.757	1.00	27.36	6
ATOM	1081	CB	ALA	A	138	30.149	26.997	42.645	1.00	27.57	6
ATOM	1082	C	ALA	A	138	28.496	26.003	44.213	1.00	26.45	6
ATOM	1083	O	ALA	A	138	27.747	25.083	43.865	1.00	27.30	8
ATOM	1084	N	ASN	A	139	28.090	27.021	44.975	1.00	22.47	7
ATOM	1085	CA	ASN	A	139	26.711	27.063	45.471	1.00	23.85	6
ATOM	1086	CB	ASN	A	139	26.406	25.738	46.218	1.00	16.82	6
ATOM	1087	CG	ASN	A	139	25.040	25.718	46.900	1.00	14.45	6
ATOM	1088	OD1	ASN	A	139	24.019	26.084	46.319	1.00	13.39	8
ATOM	1089	ND2	ASN	A	139	25.018	25.249	48.139	1.00	20.08	7
ATOM	1090	C	ASN	A	139	26.444	28.277	46.368	1.00	26.09	6
ATOM	1091	O	ASN	A	139	27.239	28.600	47.260	1.00	27.50	8
ATOM	1092	N	GLY	A	140	25.326	28.954	46.114	1.00	24.83	7
ATOM	1093	CA	GLY	A	140	24.965	30.106	46.916	1.00	22.24	6
ATOM	1094	C	GLY	A	140	25.991	31.211	46.890	1.00	22.35	6
ATOM	1095	O	GLY	A	140	26.256	31.843	47.910	1.00	23.50	8
ATOM	1096	N	PHE	A	141	26.570	31.437	45.717	1.00	25.60	7
ATOM	1097	CA	PHE	A	141	27.582	32.476	45.518	1.00	26.47	6
ATOM	1098	CB	PHE	A	141	27.204	33.765	46.258	1.00	28.05	6
ATOM	1099	CG	PHE	A	141	25.925	34.391	45.792	1.00	28.61	6
ATOM	1100	CD1	PHE	A	141	25.352	35.428	46.518	1.00	30.74	6
ATOM	1101	CD2	PHE	A	141	25.312	33.975	44.620	1.00	29.10	6
ATOM	1102	CE1	PHE	A	141	24.193	36.044	46.087	1.00	29.33	6
ATOM	1103	CE2	PHE	A	141	24.150	34.583	44.177	1.00	31.03	6
ATOM	1104	CZ	PHE	A	141	23.589	35.621	44.912	1.00	32.59	6
ATOM	1105	C	PHE	A	141	28.954	32.038	45.991	1.00	24.63	6
ATOM	1106	O	PHE	A	141	29.938	32.727	45.733	1.00	29.72	8
ATOM	1107	N	CYS	A	142	29.025	30.897	46.667	1.00	21.11	7
ATOM	1108	CA	CYS	A	142	30.296	30.399	47.192	1.00	22.30	6
ATOM	1109	CB	CYS	A	142	30.062	29.787	48.567	1.00	21.31	6
ATOM	1110	SG	CYS	A	142	28.943	30.748	49.582	1.00	22.93	16
ATOM	1111	C	CYS	A	142	31.017	29.366	46.326	1.00	22.13	6
ATOM	1112	O	CYS	A	142	30.408	28.389	45.878	1.00	22.97	8
ATOM	1113	N	TYR	A	143	32.317	29.573	46.111	1.00	23.09	7
ATOM	1114	CA	TYR	A	143	33.129	28.632	45.335	1.00	23.05	6
ATOM	1115	CB	TYR	A	143	34.063	29.365	44.375	1.00	21.60	6
ATOM	1116	CG	TYR	A	143	33.377	30.379	43.487	1.00	24.09	6
ATOM	1117	CD1	TYR	A	143	32.969	31.609	43.999	1.00	23.29	6
ATOM	1118	CE1	TYR	A	143	32.365	32.555	43.199	1.00	23.26	6
ATOM	1119	CD2	TYR	A	143	33.154	30.117	42.135	1.00	22.52	6
ATOM	1120	CE2	TYR	A	143	32.544	31.061	41.517	1.00	24.82	6
ATOM	1121	CZ	TYR	A	143	32.153	32.281	41.857	1.00	27.55	6
ATOM	1122	OH	TYR	A	143	31.553	33.241	41.064	1.00	32.35	8

Figure 17-18

ATOM	1123	C	TYR A 143	33.960	27.766	46.290	1.00	24.22	6
ATOM	1124	O	TYR A 143	34.266	26.606	45.998	1.00	24.58	8
ATOM	1125	N	ILE A 144	34.327	28.329	47.437	1.00	23.83	7
ATOM	1126	CA	ILE A 144	35.086	27.566	48.425	1.00	20.24	6
ATOM	1127	CB	ILE A 144	36.547	27.982	48.453	1.00	17.27	6
ATOM	1128	CG2	ILE A 144	37.231	27.354	49.662	1.00	11.03	6
ATOM	1129	CG1	ILE A 144	37.185	27.603	47.110	1.00	14.93	6
ATOM	1130	CD1	ILE A 144	38.601	28.028	46.946	1.00	19.68	6
ATOM	1131	C	ILE A 144	34.495	27.703	49.815	1.00	21.77	6
ATOM	1132	O	ILE A 144	34.288	28.811	50.318	1.00	21.19	8
ATOM	1133	N	ASN A 145	34.212	26.555	50.424	1.00	23.00	7
ATOM	1134	CA	ASN A 145	33.616	26.508	51.750	1.00	20.92	6
ATOM	1135	CB	ASN A 145	32.902	25.170	51.935	1.00	17.08	6
ATOM	1136	CG	ASN A 145	32.079	25.125	53.203	1.00	21.04	6
ATOM	1137	OD1	ASN A 145	32.549	25.508	54.276	1.00	20.97	8
ATOM	1138	ND2	ASN A 145	30.844	24.640	53.093	1.00	20.93	7
ATOM	1139	C	ASN A 145	34.706	26.669	52.806	1.00	19.68	6
ATOM	1140	O	ASN A 145	35.201	25.679	53.351	1.00	20.64	8
ATOM	1141	N	ASN A 146	35.079	27.911	53.100	1.00	16.28	7
ATOM	1142	CA	ASN A 146	36.123	28.143	54.088	1.00	19.34	6
ATOM	1143	CB	ASN A 146	36.428	29.651	54.207	1.00	20.27	6
ATOM	1144	CG	ASN A 146	35.292	30.444	54.795	1.00	18.05	6
ATOM	1145	OD1	ASN A 146	35.079	30.421	55.999	1.00	25.83	8
ATOM	1146	ND2	ASN A 146	34.552	31.149	53.948	1.00	16.04	7
ATOM	1147	C	ASN A 146	35.775	27.504	55.443	1.00	20.48	6
ATOM	1148	O	ASN A 146	36.663	27.027	56.151	1.00	19.88	8
ATOM	1149	N	PRO A 147	34.482	27.485	55.819	1.00	19.38	7
ATOM	1150	CD	PRO A 147	33.312	28.068	55.135	1.00	17.48	6
ATOM	1151	CA	PRO A 147	34.058	26.877	57.087	1.00	22.25	6
ATOM	1152	CB	PRO A 147	32.539	27.065	57.057	1.00	20.15	6
ATOM	1153	CG	PRO A 147	32.407	28.378	56.305	1.00	20.81	6
ATOM	1154	C	PRO A 147	34.443	25.383	57.188	1.00	26.89	6
ATOM	1155	O	PRO A 147	35.066	24.954	58.169	1.00	29.10	8
ATOM	1156	N	ALA A 148	34.070	24.596	56.176	1.00	25.88	7
ATOM	1157	CA	ALA A 148	34.372	23.164	56.174	1.00	25.47	6
ATOM	1158	CB	ALA A 148	33.670	22.468	55.009	1.00	21.84	6
ATOM	1159	C	ALA A 148	35.870	22.916	56.100	1.00	25.94	6
ATOM	1160	O	ALA A 148	36.382	21.971	56.701	1.00	27.19	8
ATOM	1161	N	VAL A 149	36.574	23.756	55.349	1.00	26.11	7
ATOM	1162	CA	VAL A 149	38.017	23.609	55.233	1.00	24.04	6
ATOM	1163	CB	VAL A 149	38.622	24.663	54.267	1.00	26.16	6
ATOM	1164	CG1	VAL A 149	40.135	24.476	54.158	1.00	25.36	6
ATOM	1165	CG2	VAL A 149	37.970	24.544	52.886	1.00	26.81	6
ATOM	1166	C	VAL A 149	38.516	23.870	56.640	1.00	23.57	6
ATOM	1167	O	VAL A 149	39.453	23.228	57.122	1.00	19.75	8
ATOM	1168	N	GLY A 150	37.850	24.815	57.299	1.00	22.20	7
ATOM	1169	CA	GLY A 150	38.210	25.175	58.654	1.00	25.43	6
ATOM	1170	C	GLY A 150	38.130	23.975	59.568	1.00	27.19	6
ATOM	1171	O	GLY A 150	39.112	23.620	60.221	1.00	27.05	8
ATOM	1172	N	ILE A 151	36.959	23.348	59.618	1.00	25.56	7
ATOM	1173	CA	ILE A 151	36.775	22.176	60.457	1.00	28.24	6
ATOM	1174	CB	ILE A 151	35.317	21.654	60.389	1.00	29.41	6
ATOM	1175	CG2	ILE A 151	35.251	20.215	60.869	1.00	26.02	6
ATOM	1176	CG1	ILE A 151	34.394	22.540	61.240	1.00	33.31	6
ATOM	1177	CD1	ILE A 151	34.255	23.967	60.759	1.00	36.83	6
ATOM	1178	C	ILE A 151	37.723	21.039	60.075	1.00	29.32	6
ATOM	1179	O	ILE A 151	38.340	20.420	60.947	1.00	29.08	8
ATOM	1180	N	GLU A 152	37.843	20.769	58.778	1.00	29.91	7
ATOM	1181	CA	GLU A 152	38.704	19.690	58.315	1.00	32.58	6
ATOM	1182	CB	GLU A 152	38.575	19.526	56.802	1.00	35.07	6
ATOM	1183	CG	GLU A 152	37.269	18.848	56.393	1.00	38.51	6
ATOM	1184	CD	GLU A 152	37.120	17.440	56.987	1.00	41.41	6
ATOM	1185	OE1	GLU A 152	36.089	16.779	56.718	1.00	45.64	8
ATOM	1186	OE2	GLU A 152	38.030	16.992	57.723	1.00	40.09	8
ATOM	1187	C	GLU A 152	40.145	19.903	58.721	1.00	32.97	6
ATOM	1188	O	GLU A 152	40.879	18.946	58.978	1.00	30.15	8

86/263

Figure 17-19

ATOM	1189	N	TYR	A	153	40.541	21.170	58.765	1.00	33.90	7
ATOM	1190	CA	TYR	A	153	41.875	21.563	59.193	1.00	32.04	6
ATOM	1191	CB	TYR	A	153	42.019	23.074	59.058	1.00	34.88	6
ATOM	1192	CG	TYR	A	153	43.280	23.667	59.639	1.00	38.03	6
ATOM	1193	CD1	TYR	A	153	44.498	23.611	58.948	1.00	42.34	6
ATOM	1194	CE1	TYR	A	153	45.658	24.207	59.475	1.00	43.38	6
ATOM	1195	CD2	TYR	A	153	43.250	24.321	60.869	1.00	37.19	6
ATOM	1196	CE2	TYR	A	153	44.387	24.913	61.401	1.00	41.09	6
ATOM	1197	CZ	TYR	A	153	45.587	24.860	60.704	1.00	43.34	6
ATOM	1198	OH	TYR	A	153	46.696	25.480	61.241	1.00	44.86	8
ATOM	1199	C	TYR	A	153	41.919	21.168	60.667	1.00	32.59	6
ATOM	1200	O	TYR	A	153	42.867	20.518	61.120	1.00	32.24	8
ATOM	1201	N	LEU	A	154	40.869	21.556	61.397	1.00	30.10	7
ATOM	1202	CA	LEU	A	154	40.730	21.261	62.823	1.00	29.38	6
ATOM	1203	CB	LEU	A	154	39.443	21.889	63.378	1.00	28.60	6
ATOM	1204	CG	LEU	A	154	39.399	23.407	63.618	1.00	31.20	6
ATOM	1205	CD1	LEU	A	154	37.991	23.833	64.041	1.00	28.53	6
ATOM	1206	CD2	LEU	A	154	40.418	23.787	64.691	1.00	24.95	6
ATOM	1207	C	LEU	A	154	40.732	19.772	63.146	1.00	29.56	6
ATOM	1208	O	LEU	A	154	41.223	19.363	64.196	1.00	28.36	8
ATOM	1209	N	ARG	A	155	40.174	18.958	62.256	1.00	31.95	7
ATOM	1210	CA	ARG	A	155	40.134	17.522	62.499	1.00	33.00	6
ATOM	1211	CB	ARG	A	155	39.127	16.847	61.561	1.00	33.13	6
ATOM	1212	CG	ARG	A	155	37.708	17.368	61.769	1.00	32.84	6
ATOM	1213	CD	ARG	A	155	36.678	16.719	60.863	1.00	32.92	6
ATOM	1214	NE	ARG	A	155	36.152	15.451	61.363	1.00	33.98	7
ATOM	1215	CZ	ARG	A	155	35.195	14.760	60.741	1.00	37.93	6
ATOM	1216	NH1	ARG	A	155	34.671	15.216	59.605	1.00	38.39	7
ATOM	1217	NH2	ARG	A	155	34.732	13.631	61.259	1.00	38.67	7
ATOM	1218	C	ARG	A	155	41.521	16.929	62.331	1.00	33.97	6
ATOM	1219	O	ARG	A	155	41.869	15.941	62.985	1.00	32.95	8
ATOM	1220	N	LYS	A	156	42.318	17.548	61.467	1.00	34.20	7
ATOM	1221	CA	LYS	A	156	43.679	17.081	61.243	1.00	36.32	6
ATOM	1222	CB	LYS	A	156	44.249	17.662	59.942	1.00	37.57	6
ATOM	1223	CG	LYS	A	156	45.673	17.187	59.638	1.00	40.32	6
ATOM	1224	CD	LYS	A	156	46.116	17.532	58.220	1.00	40.33	6
ATOM	1225	CE	LYS	A	156	45.180	16.909	57.184	1.00	41.27	6
ATOM	1226	NZ	LYS	A	156	45.015	15.435	57.364	1.00	37.92	7
ATOM	1227	C	LYS	A	156	44.539	17.501	62.428	1.00	36.17	6
ATOM	1228	O	LYS	A	156	45.582	16.905	62.699	1.00	34.53	8
ATOM	1229	N	LYS	A	157	44.093	18.537	63.132	1.00	36.71	7
ATOM	1230	CA	LYS	A	157	44.820	19.026	64.294	1.00	37.09	6
ATOM	1231	CB	LYS	A	157	44.495	20.501	64.566	1.00	37.02	6
ATOM	1232	CG	LYS	A	157	44.982	21.435	63.477	1.00	36.22	6
ATOM	1233	CD	LYS	A	157	46.468	21.231	63.239	1.00	37.91	6
ATOM	1234	CE	LYS	A	157	46.993	22.100	62.107	1.00	39.35	6
ATOM	1235	NZ	LYS	A	157	48.434	21.815	61.842	1.00	38.78	7
ATOM	1236	C	LYS	A	157	44.498	18.178	65.515	1.00	35.61	6
ATOM	1237	O	LYS	A	157	45.204	18.232	66.518	1.00	36.38	8
ATOM	1238	N	GLY	A	158	43.433	17.392	65.431	1.00	34.37	7
ATOM	1239	CA	GLY	A	158	43.097	16.537	66.552	1.00	38.08	6
ATOM	1240	C	GLY	A	158	41.782	16.781	67.267	1.00	38.78	6
ATOM	1241	O	GLY	A	158	41.460	16.053	68.208	1.00	41.07	8
ATOM	1242	N	PHE	A	159	41.023	17.791	66.855	1.00	36.75	7
ATOM	1243	CA	PHE	A	159	39.743	18.046	67.505	1.00	33.83	6
ATOM	1244	CB	PHE	A	159	39.246	19.459	67.213	1.00	32.65	6
ATOM	1245	CG	PHE	A	159	40.115	20.521	67.787	1.00	29.97	6
ATOM	1246	CD1	PHE	A	159	41.404	20.724	67.297	1.00	30.20	6
ATOM	1247	CD2	PHE	A	159	39.672	21.289	68.853	1.00	29.28	6
ATOM	1248	CE1	PHE	A	159	42.241	21.680	67.862	1.00	28.96	6
ATOM	1249	CE2	PHE	A	159	40.498	22.246	69.428	1.00	29.67	6
ATOM	1250	CZ	PHE	A	159	41.785	22.442	68.931	1.00	30.59	6
ATOM	1251	C	PHE	A	159	38.732	17.026	67.025	1.00	33.41	6
ATOM	1252	O	PHE	A	159	38.664	16.716	65.838	1.00	31.61	8
ATOM	1253	N	LYS	A	160	37.951	16.506	67.966	1.00	35.13	7
ATOM	1254	CA	LYS	A	160	36.947	15.493	67.677	1.00	35.39	6

Figure 17-20

ATOM	1255	CB	LYS	A	160	37.342	14.198	68.389	1.00	36.43	6
ATOM	1256	CG	LYS	A	160	38.535	13.502	67.708	1.00	40.67	6
ATOM	1257	CD	LYS	A	160	39.312	12.538	68.615	1.00	44.68	6
ATOM	1258	CE	LYS	A	160	38.425	11.536	69.345	1.00	49.23	6
ATOM	1259	NZ	LYS	A	160	37.593	12.182	70.411	1.00	50.63	7
ATOM	1260	C	LYS	A	160	35.524	15.927	68.027	1.00	35.94	6
ATOM	1261	O	LYS	A	160	34.561	15.241	67.691	1.00	35.72	8
ATOM	1262	N	ARG	A	161	35.399	17.058	68.718	1.00	34.35	7
ATOM	1263	CA	ARG	A	161	34.091	17.618	69.044	1.00	34.95	6
ATOM	1264	CB	ARG	A	161	33.771	17.525	70.535	1.00	33.94	6
ATOM	1265	CG	ARG	A	161	33.427	16.132	70.992	1.00	38.25	6
ATOM	1266	CD	ARG	A	161	32.823	16.131	72.386	1.00	41.17	6
ATOM	1267	NE	ARG	A	161	33.719	16.722	73.378	1.00	47.64	7
ATOM	1268	CZ	ARG	A	161	34.912	16.233	73.705	1.00	47.92	6
ATOM	1269	NH1	ARG	A	161	35.372	15.131	73.121	1.00	47.56	7
ATOM	1270	NH2	ARG	A	161	35.648	16.858	74.616	1.00	46.95	7
ATOM	1271	C	ARG	A	161	34.113	19.076	68.598	1.00	34.58	6
ATOM	1272	O	ARG	A	161	34.468	19.980	69.357	1.00	33.77	8
ATOM	1273	N	ILE	A	162	33.741	19.280	67.341	1.00	31.74	7
ATOM	1274	CA	ILE	A	162	33.735	20.594	66.735	1.00	29.83	6
ATOM	1275	CB	ILE	A	162	34.429	20.542	65.362	1.00	29.96	6
ATOM	1276	CG2	ILE	A	162	34.580	21.942	64.784	1.00	30.57	6
ATOM	1277	CG1	ILE	A	162	35.801	19.891	65.522	1.00	28.81	6
ATOM	1278	CD1	ILE	A	162	36.537	19.685	64.224	1.00	33.05	6
ATOM	1279	C	ILE	A	162	32.300	21.050	66.560	1.00	29.66	6
ATOM	1280	O	ILE	A	162	31.416	20.241	66.266	1.00	25.24	8
ATOM	1281	N	LEU	A	163	32.081	22.351	66.745	1.00	30.00	7
ATOM	1282	CA	LEU	A	163	30.754	22.945	66.617	1.00	30.48	6
ATOM	1283	CB	LEU	A	163	30.236	23.406	67.992	1.00	32.25	6
ATOM	1284	CG	LEU	A	163	28.934	24.229	68.044	1.00	31.21	6
ATOM	1285	CD1	LEU	A	163	27.804	23.494	67.326	1.00	31.58	6
ATOM	1286	CD2	LEU	A	163	28.569	24.502	69.493	1.00	25.00	6
ATOM	1287	C	LEU	A	163	30.717	24.122	65.659	1.00	29.23	6
ATOM	1288	O	LEU	A	163	31.596	24.980	65.654	1.00	29.72	8
ATOM	1289	N	TYR	A	164	29.675	24.157	64.846	1.00	29.68	7
ATOM	1290	CA	TYR	A	164	29.500	25.244	63.899	1.00	29.89	6
ATOM	1291	CB	TYR	A	164	29.512	24.688	62.470	1.00	27.81	6
ATOM	1292	CG	TYR	A	164	29.377	25.742	61.399	1.00	27.79	6
ATOM	1293	CD1	TYR	A	164	30.390	26.670	61.168	1.00	24.82	6
ATOM	1294	CE1	TYR	A	164	30.247	27.655	60.198	1.00	24.51	6
ATOM	1295	CD2	TYR	A	164	28.216	25.827	60.631	1.00	27.61	6
ATOM	1296	CE2	TYR	A	164	28.065	26.808	59.662	1.00	25.67	6
ATOM	1297	CZ	TYR	A	164	29.078	27.718	59.451	1.00	25.63	6
ATOM	1298	OH	TYR	A	164	28.898	28.704	58.506	1.00	27.10	8
ATOM	1299	C	TYR	A	164	28.149	25.907	64.218	1.00	28.38	6
ATOM	1300	O	TYR	A	164	27.119	25.225	64.277	1.00	29.43	8
ATOM	1301	N	ILE	A	165	28.166	27.217	64.464	1.00	24.30	7
ATOM	1302	CA	ILE	A	165	26.941	27.969	64.754	1.00	22.93	6
ATOM	1303	CB	ILE	A	165	26.985	28.649	66.143	1.00	22.00	6
ATOM	1304	CG2	ILE	A	165	25.765	29.559	66.312	1.00	16.15	6
ATOM	1305	CG1	ILE	A	165	27.033	27.567	67.240	1.00	20.78	6
ATOM	1306	CD1	ILE	A	165	27.185	28.101	68.650	1.00	15.49	6
ATOM	1307	C	ILE	A	165	26.784	29.010	63.657	1.00	24.45	6
ATOM	1308	O	ILE	A	165	27.605	29.921	63.506	1.00	23.17	8
ATOM	1309	N	ASP	A	166	25.709	28.871	62.895	1.00	24.20	7
ATOM	1310	CA	ASP	A	166	25.478	29.726	61.749	1.00	20.78	6
ATOM	1311	CB	ASP	A	166	25.314	28.809	60.548	1.00	17.64	6
ATOM	1312	CG	ASP	A	166	25.410	29.529	59.256	1.00	19.93	6
ATOM	1313	OD1	ASP	A	166	24.536	30.391	59.004	1.00	20.20	8
ATOM	1314	OD2	ASP	A	166	26.366	29.231	58.491	1.00	17.64	8
ATOM	1315	C	ASP	A	166	24.290	30.670	61.895	1.00	22.79	6
ATOM	1316	O	ASP	A	166	23.134	30.256	61.826	1.00	22.70	8
ATOM	1317	N	LEU	A	167	24.583	31.952	62.085	1.00	25.40	7
ATOM	1318	CA	LEU	A	167	23.536	32.954	62.250	1.00	25.76	6
ATOM	1319	CB	LEU	A	167	23.963	33.991	63.288	1.00	26.65	6
ATOM	1320	CG	LEU	A	167	24.364	33.463	64.674	1.00	26.75	6

Figure 17-21

ATOM	1321	CD1	LEU	A	167	24.741	34.647	65.552	1.00	26.24	6
ATOM	1322	CD2	LEU	A	167	23.225	32.661	65.302	1.00	23.45	6
ATOM	1323	C	LEU	A	167	23.162	33.660	60.951	1.00	26.37	6
ATOM	1324	O	LEU	A	167	22.386	34.613	60.971	1.00	25.95	8
ATOM	1325	N	ASP	A	168	23.726	33.208	59.828	1.00	29.66	7
ATOM	1326	CA	ASP	A	168	23.410	33.787	58.520	1.00	28.35	6
ATOM	1327	CB	ASP	A	168	24.057	32.987	57.390	1.00	33.29	6
ATOM	1328	CG	ASP	A	168	23.937	33.676	56.037	1.00	35.38	6
ATOM	1329	OD1	ASP	A	168	24.892	34.388	55.659	1.00	39.48	8
ATOM	1330	OD2	ASP	A	168	22.893	33.531	55.364	1.00	33.40	8
ATOM	1331	C	ASP	A	168	21.906	33.614	58.408	1.00	28.74	6
ATOM	1332	O	ASP	A	168	21.354	32.648	58.948	1.00	26.21	8
ATOM	1333	N	ALA	A	169	21.239	34.524	57.711	1.00	26.16	7
ATOM	1334	CA	ALA	A	169	19.793	34.415	57.579	1.00	24.39	6
ATOM	1335	CB	ALA	A	169	19.233	35.640	56.879	1.00	22.75	6
ATOM	1336	C	ALA	A	169	19.420	33.157	56.813	1.00	24.37	6
ATOM	1337	O	ALA	A	169	18.266	32.752	56.824	1.00	22.34	8
ATOM	1338	N	HIS	A	170	20.405	32.542	56.156	1.00	25.78	7
ATOM	1339	CA	HIS	A	170	20.180	31.327	55.375	1.00	25.20	6
ATOM	1340	CB	HIS	A	170	20.667	31.501	53.936	1.00	25.76	6
ATOM	1341	CG	HIS	A	170	20.122	32.711	53.245	1.00	29.08	6
ATOM	1342	CD2	HIS	A	170	19.338	32.834	52.147	1.00	30.59	6
ATOM	1343	ND1	HIS	A	170	20.384	33.995	53.675	1.00	30.77	7
ATOM	1344	CE1	HIS	A	170	19.784	34.858	52.873	1.00	29.07	6
ATOM	1345	NE2	HIS	A	170	19.143	34.180	51.939	1.00	32.19	7
ATOM	1346	C	HIS	A	170	20.895	30.113	55.958	1.00	26.00	6
ATOM	1347	O	HIS	A	170	21.913	30.234	56.637	1.00	25.76	8
ATOM	1348	N	HIS	A	171	20.349	28.939	55.658	1.00	27.29	7
ATOM	1349	CA	HIS	A	171	20.893	27.655	56.090	1.00	25.01	6
ATOM	1350	CB	HIS	A	171	19.934	26.532	55.663	1.00	24.93	6
ATOM	1351	CG	HIS	A	171	20.468	25.148	55.889	1.00	26.56	6
ATOM	1352	CD2	HIS	A	171	20.674	24.123	55.028	1.00	22.34	6
ATOM	1353	ND1	HIS	A	171	20.823	24.678	57.137	1.00	25.35	7
ATOM	1354	CE1	HIS	A	171	21.222	23.424	57.036	1.00	22.68	6
ATOM	1355	NE2	HIS	A	171	21.140	23.062	55.767	1.00	24.13	7
ATOM	1356	C	HIS	A	171	22.267	27.413	55.471	1.00	24.74	6
ATOM	1357	O	HIS	A	171	22.540	27.863	54.356	1.00	28.22	8
ATOM	1358	N	CYS	A	172	23.131	26.705	56.190	1.00	23.03	7
ATOM	1359	CA	CYS	A	172	24.467	26.389	55.683	1.00	23.41	6
ATOM	1360	CB	CYS	A	172	25.497	26.474	56.812	1.00	19.31	6
ATOM	1361	SG	CYS	A	172	25.005	25.631	58.318	1.00	16.78	16
ATOM	1362	C	CYS	A	172	24.484	24.997	55.048	1.00	25.45	6
ATOM	1363	O	CYS	A	172	25.203	24.098	55.483	1.00	24.47	8
ATOM	1364	N	ASP	A	173	23.664	24.839	54.015	1.00	26.67	7
ATOM	1365	CA	ASP	A	173	23.542	23.593	53.269	1.00	26.47	6
ATOM	1366	CB	ASP	A	173	22.735	23.857	51.993	1.00	26.33	6
ATOM	1367	CG	ASP	A	173	23.281	25.030	51.179	1.00	27.06	6
ATOM	1368	OD1	ASP	A	173	22.539	25.558	50.330	1.00	23.43	8
ATOM	1369	OD2	ASP	A	173	24.454	25.417	51.372	1.00	29.38	8
ATOM	1370	C	ASP	A	173	24.872	22.932	52.922	1.00	26.65	6
ATOM	1371	O	ASP	A	173	24.940	21.708	52.784	1.00	28.38	8
ATOM	1372	N	GLY	A	174	25.926	23.737	52.793	1.00	25.24	7
ATOM	1373	CA	GLY	A	174	27.227	23.198	52.447	1.00	23.11	6
ATOM	1374	C	GLY	A	174	27.896	22.505	53.612	1.00	25.64	6
ATOM	1375	O	GLY	A	174	28.443	21.408	53.462	1.00	27.67	8
ATOM	1376	N	VAL	A	175	27.848	23.144	54.778	1.00	24.29	7
ATOM	1377	CA	VAL	A	175	28.459	22.602	55.989	1.00	22.20	6
ATOM	1378	CB	VAL	A	175	28.536	23.672	57.101	1.00	20.15	6
ATOM	1379	CG1	VAL	A	175	29.449	23.192	58.218	1.00	20.11	6
ATOM	1380	CG2	VAL	A	175	29.015	24.989	56.530	1.00	18.74	6
ATOM	1381	C	VAL	A	175	27.647	21.409	56.505	1.00	22.85	6
ATOM	1382	O	VAL	A	175	28.173	20.512	57.173	1.00	20.07	8
ATOM	1383	N	GLN	A	176	26.356	21.404	56.203	1.00	24.12	7
ATOM	1384	CA	GLN	A	176	25.518	20.303	56.629	1.00	27.18	6
ATOM	1385	CB	GLN	A	176	24.045	20.611	56.355	1.00	32.86	6
ATOM	1386	CG	GLN	A	176	23.084	19.483	56.726	1.00	36.04	6

ATOM	1387	CD	GLN	A	176	21.620	19.862	56.537	1.00	38.36	6
ATOM	1388	OE1	GLN	A	176	21.113	20.782	57.185	1.00	38.59	8
ATOM	1389	NE2	GLN	A	176	20.934	19.151	55.649	1.00	38.81	7
ATOM	1390	C	GLN	A	176	25.956	19.083	55.841	1.00	27.70	6
ATOM	1391	O	GLN	A	176	26.326	18.066	56.416	1.00	26.89	8
ATOM	1392	N	GLU	A	177	25.951	19.194	54.519	1.00	27.96	7
ATOM	1393	CA	GLU	A	177	26.343	18.062	53.698	1.00	31.16	6
ATOM	1394	CB	GLU	A	177	26.395	18.460	52.220	1.00	30.37	6
ATOM	1395	CG	GLU	A	177	26.353	17.256	51.287	1.00	36.20	6
ATOM	1396	CD	GLU	A	177	26.273	17.626	49.818	1.00	40.70	6
ATOM	1397	OE1	GLU	A	177	27.322	17.967	49.234	1.00	46.78	8
ATOM	1398	OE2	GLU	A	177	25.155	17.590	49.250	1.00	39.39	8
ATOM	1399	C	GLU	A	177	27.702	17.516	54.137	1.00	31.66	6
ATOM	1400	O	GLU	A	177	27.868	16.317	54.356	1.00	32.81	8
ATOM	1401	N	ALA	A	178	28.663	18.419	54.287	1.00	33.39	7
ATOM	1402	CA	ALA	A	178	30.026	18.072	54.673	1.00	31.63	6
ATOM	1403	CB	ALA	A	178	30.830	19.338	54.856	1.00	30.96	6
ATOM	1404	C	ALA	A	178	30.204	17.185	55.897	1.00	30.63	6
ATOM	1405	O	ALA	A	178	31.032	16.276	55.876	1.00	27.95	8
ATOM	1406	N	PHE	A	179	29.444	17.444	56.961	1.00	31.01	7
ATOM	1407	CA	PHE	A	179	29.590	16.656	58.184	1.00	31.34	6
ATOM	1408	CB	PHE	A	179	30.147	17.532	59.310	1.00	30.13	6
ATOM	1409	CG	PHE	A	179	31.189	18.505	58.858	1.00	27.78	6
ATOM	1410	CD1	PHE	A	179	30.827	19.790	58.466	1.00	28.24	6
ATOM	1411	CD2	PHE	A	179	32.522	18.124	58.766	1.00	28.33	6
ATOM	1412	CE1	PHE	A	179	31.778	20.688	57.988	1.00	26.68	6
ATOM	1413	CE2	PHE	A	179	33.487	19.013	58.285	1.00	28.79	6
ATOM	1414	CZ	PHE	A	179	33.111	20.300	57.895	1.00	28.67	6
ATOM	1415	C	PHE	A	179	28.300	16.003	58.664	1.00	32.06	6
ATOM	1416	O	PHE	A	179	28.218	15.542	59.803	1.00	30.58	8
ATOM	1417	N	TYR	A	180	27.305	15.960	57.787	1.00	34.25	7
ATOM	1418	CA	TYR	A	180	26.001	15.377	58.099	1.00	38.60	6
ATOM	1419	CB	TYR	A	180	25.062	15.605	56.911	1.00	38.99	6
ATOM	1420	CG	TYR	A	180	23.593	15.453	57.220	1.00	37.91	6
ATOM	1421	CD1	TYR	A	180	22.938	14.232	57.064	1.00	35.83	6
ATOM	1422	CE1	TYR	A	180	21.589	14.103	57.373	1.00	39.20	6
ATOM	1423	CD2	TYR	A	180	22.861	16.543	57.694	1.00	37.56	6
ATOM	1424	CE2	TYR	A	180	21.518	16.430	58.007	1.00	40.28	6
ATOM	1425	CZ	TYR	A	180	20.882	15.211	57.848	1.00	41.92	6
ATOM	1426	OH	TYR	A	180	19.549	15.110	58.188	1.00	43.41	8
ATOM	1427	C	TYR	A	180	26.133	13.884	58.382	1.00	40.28	6
ATOM	1428	O	TYR	A	180	25.158	13.192	58.680	1.00	39.27	8
ATOM	1429	N	ASP	A	181	27.363	13.402	58.319	1.00	43.51	7
ATOM	1430	CA	ASP	A	181	27.638	11.994	58.519	1.00	45.89	6
ATOM	1431	CB	ASP	A	181	28.414	11.487	57.303	1.00	51.00	6
ATOM	1432	CG	ASP	A	181	28.830	10.050	57.436	1.00	56.84	6
ATOM	1433	OD1	ASP	A	181	29.637	9.750	58.345	1.00	59.47	8
ATOM	1434	OD2	ASP	A	181	28.348	9.221	56.629	1.00	60.73	8
ATOM	1435	C	ASP	A	181	28.398	11.665	59.804	1.00	44.75	6
ATOM	1436	O	ASP	A	181	28.257	10.568	60.350	1.00	44.69	8
ATOM	1437	N	THR	A	182	29.194	12.606	60.298	1.00	41.26	7
ATOM	1438	CA	THR	A	182	29.975	12.337	61.495	1.00	39.51	6
ATOM	1439	CB	THR	A	182	31.408	12.881	61.355	1.00	39.19	6
ATOM	1440	OG1	THR	A	182	32.171	12.508	62.505	1.00	37.82	8
ATOM	1441	CG2	THR	A	182	31.395	14.397	61.232	1.00	40.12	6
ATOM	1442	C	THR	A	182	29.370	12.910	62.759	1.00	38.58	6
ATOM	1443	O	THR	A	182	28.609	13.876	62.716	1.00	41.24	8
ATOM	1444	N	ASP	A	183	29.712	12.304	63.890	1.00	37.39	7
ATOM	1445	CA	ASP	A	183	29.211	12.773	65.171	1.00	39.24	6
ATOM	1446	CB	ASP	A	183	28.824	11.588	66.061	1.00	40.31	6
ATOM	1447	CG	ASP	A	183	30.010	10.723	66.433	1.00	41.64	6
ATOM	1448	OD1	ASP	A	183	30.725	10.268	65.520	1.00	42.53	8
ATOM	1449	OD2	ASP	A	183	30.221	10.494	67.640	1.00	42.46	8
ATOM	1450	C	ASP	A	183	30.286	13.621	65.853	1.00	40.34	6
ATOM	1451	O	ASP	A	183	30.109	14.071	66.983	1.00	42.07	8
ATOM	1452	N	GLN	A	184	31.400	13.830	65.154	1.00	39.29	7

ATOM	1453	CA	GLN	A	184	32.506	14.635	65.671	1.00	37.08	6
ATOM	1454	CB	GLN	A	184	33.830	14.252	64.994	1.00	33.77	6
ATOM	1455	CG	GLN	A	184	34.229	12.804	65.166	1.00	33.63	6
ATOM	1456	CD	GLN	A	184	35.599	12.499	64.593	1.00	32.74	6
ATOM	1457	OE1	GLN	A	184	35.853	12.704	63.413	1.00	31.17	8
ATOM	1458	NE2	GLN	A	184	36.490	11.999	65.436	1.00	36.58	7
ATOM	1459	C	GLN	A	184	32.222	16.110	65.403	1.00	36.42	6
ATOM	1460	O	GLN	A	184	32.803	16.994	66.034	1.00	37.41	8
ATOM	1461	N	VAL	A	185	31.329	16.372	64.456	1.00	33.14	7
ATOM	1462	CA	VAL	A	185	30.984	17.740	64.119	1.00	32.40	6
ATOM	1463	CB	VAL	A	185	31.308	18.052	62.641	1.00	33.03	6
ATOM	1464	CG1	VAL	A	185	31.009	19.520	62.331	1.00	29.27	6
ATOM	1465	CG2	VAL	A	185	32.773	17.738	62.357	1.00	34.58	6
ATOM	1466	C	VAL	A	185	29.508	17.972	64.360	1.00	31.51	6
ATOM	1467	O	VAL	A	185	28.680	17.124	64.038	1.00	31.71	8
ATOM	1468	N	PHE	A	186	29.185	19.119	64.946	1.00	30.98	7
ATOM	1469	CA	PHE	A	186	27.798	19.463	65.207	1.00	31.44	6
ATOM	1470	CB	PHE	A	186	27.524	19.532	66.716	1.00	30.96	6
ATOM	1471	CG	PHE	A	186	26.059	19.617	67.066	1.00	31.59	6
ATOM	1472	CD1	PHE	A	186	25.552	18.901	68.153	1.00	30.54	6
ATOM	1473	CD2	PHE	A	186	25.179	20.395	66.308	1.00	31.50	6
ATOM	1474	CE1	PHE	A	186	24.191	18.951	68.478	1.00	33.28	6
ATOM	1475	CE2	PHE	A	186	23.815	20.457	66.622	1.00	33.04	6
ATOM	1476	CZ	PHE	A	186	23.318	19.733	67.708	1.00	32.35	6
ATOM	1477	C	PHE	A	186	27.490	20.798	64.551	1.00	30.37	6
ATOM	1478	O	PHE	A	186	28.189	21.789	64.751	1.00	31.32	8
ATOM	1479	N	VAL	A	187	26.435	20.809	63.752	1.00	31.14	7
ATOM	1480	CA	VAL	A	187	26.024	22.015	63.063	1.00	32.05	6
ATOM	1481	CB	VAL	A	187	26.018	21.805	61.525	1.00	33.54	6
ATOM	1482	CG1	VAL	A	187	25.574	23.081	60.813	1.00	32.07	6
ATOM	1483	CG2	VAL	A	187	27.420	21.389	61.056	1.00	35.44	6
ATOM	1484	C	VAL	A	187	24.638	22.439	63.524	1.00	31.47	6
ATOM	1485	O	VAL	A	187	23.666	21.686	63.410	1.00	29.06	8
ATOM	1486	N	LEU	A	188	24.579	23.638	64.090	1.00	29.44	7
ATOM	1487	CA	LEU	A	188	23.336	24.228	64.551	1.00	29.39	6
ATOM	1488	CB	LEU	A	188	23.433	24.665	66.009	1.00	29.62	6
ATOM	1489	CG	LEU	A	188	22.293	25.589	66.458	1.00	27.92	6
ATOM	1490	CD1	LEU	A	188	20.970	24.844	66.414	1.00	25.87	6
ATOM	1491	CD2	LEU	A	188	22.574	26.107	67.861	1.00	27.69	6
ATOM	1492	C	LEU	A	188	23.161	25.454	63.675	1.00	31.89	6
ATOM	1493	O	LEU	A	188	24.130	26.175	63.388	1.00	31.50	8
ATOM	1494	N	SER	A	189	21.929	25.700	63.250	1.00	29.93	7
ATOM	1495	CA	SER	A	189	21.682	26.831	62.390	1.00	24.65	6
ATOM	1496	CB	SER	A	189	21.873	26.411	60.942	1.00	22.40	6
ATOM	1497	OG	SER	A	189	21.585	27.485	60.083	1.00	19.12	8
ATOM	1498	C	SER	A	189	20.716	27.462	62.540	1.00	27.00	6
ATOM	1499	O	SER	A	189	19.736	26.774	62.577	1.00	26.72	8
ATOM	1500	N	LEU	A	190	20.721	28.783	62.669	1.00	27.41	7
ATOM	1501	CA	LEU	A	190	19.096	29.554	62.735	1.00	29.68	6
ATOM	1502	CB	LEU	A	190	19.185	30.682	63.771	1.00	29.84	6
ATOM	1503	CG	LEU	A	190	19.108	30.366	65.264	1.00	26.79	6
ATOM	1504	CD1	LEU	A	190	19.020	31.662	66.045	1.00	23.44	6
ATOM	1505	CD2	LEU	A	190	17.881	29.549	65.546	1.00	27.63	6
ATOM	1506	C	LEU	A	190	19.046	30.141	61.329	1.00	29.58	6
ATOM	1507	O	LEU	A	190	20.084	30.525	60.790	1.00	32.40	8
ATOM	1508	N	HIS	A	191	17.864	30.206	60.727	1.00	29.61	7
ATOM	1509	CA	HIS	A	191	17.766	30.726	59.368	1.00	29.72	6
ATOM	1510	CB	HIS	A	191	18.595	29.839	58.432	1.00	26.47	6
ATOM	1511	CG	HIS	A	191	18.225	28.392	58.504	1.00	28.18	6
ATOM	1512	CD2	HIS	A	191	18.918	27.313	58.940	1.00	28.88	6
ATOM	1513	ND1	HIS	A	191	16.989	27.921	58.118	1.00	31.00	7
ATOM	1514	CE1	HIS	A	191	16.938	26.614	58.312	1.00	30.54	6
ATOM	1515	NE2	HIS	A	191	18.095	26.220	58.810	1.00	27.21	7
ATOM	1516	C	HIS	A	191	16.329	30.812	58.856	1.00	28.05	6
ATOM	1517	O	HIS	A	191	15.385	30.411	59.535	1.00	27.81	8
ATOM	1518	N	GLN	A	192	16.183	31.346	57.649	1.00	29.39	7

Figure 17-24

ATOM	1519	CA	GLN	A	192	14.886	31.494	57.008	1.00	28.21	6
ATOM	1520	CB	GLN	A	192	15.016	32.416	55.796	1.00	24.94	6
ATOM	1521	CG	GLN	A	192	15.622	33.773	56.124	1.00	21.66	6
ATOM	1522	CD	GLN	A	192	15.701	34.690	54.921	1.00	22.22	6
ATOM	1523	OE1	GLN	A	192	14.684	35.173	54.428	1.00	23.38	8
ATOM	1524	NE2	GLN	A	192	16.914	34.925	54.434	1.00	22.97	7
ATOM	1525	C	GLN	A	192	14.435	30.104	56.570	1.00	32.71	6
ATOM	1526	O	GLN	A	192	15.157	29.403	55.853	1.00	33.85	8
ATOM	1527	N	SER	A	193	13.249	29.694	57.011	1.00	34.44	7
ATOM	1528	CA	SER	A	193	12.751	28.376	56.650	1.00	33.28	6
ATOM	1529	CB	SER	A	193	11.264	28.249	56.961	1.00	33.25	6
ATOM	1530	OG	SER	A	193	10.786	26.987	56.540	1.00	31.52	8
ATOM	1531	C	SER	A	193	12.974	28.150	55.171	1.00	34.79	6
ATOM	1532	O	SER	A	193	12.775	29.051	54.356	1.00	33.74	8
ATOM	1533	N	PRO	A	194	13.404	26.938	54.803	1.00	37.57	7
ATOM	1534	CD	PRO	A	194	13.689	25.775	55.658	1.00	38.89	6
ATOM	1535	CA	PRO	A	194	13.654	26.600	53.403	1.00	37.81	6
ATOM	1536	CB	PRO	A	194	14.248	25.194	53.498	1.00	39.30	6
ATOM	1537	CG	PRO	A	194	14.840	25.163	54.916	1.00	39.09	6
ATOM	1538	C	PRO	A	194	12.340	26.617	52.638	1.00	36.81	6
ATOM	1539	O	PRO	A	194	12.317	26.443	51.425	1.00	34.09	8
ATOM	1540	N	GLU	A	195	11.246	26.835	53.364	1.00	39.25	7
ATOM	1541	CA	GLU	A	195	9.928	26.866	52.750	1.00	41.54	6
ATOM	1542	CB	GLU	A	195	8.843	26.600	53.812	1.00	45.84	6
ATOM	1543	CG	GLU	A	195	8.360	27.811	54.608	1.00	53.30	6
ATOM	1544	CD	GLU	A	195	7.160	28.502	53.960	1.00	55.91	6
ATOM	1545	OE1	GLU	A	195	6.735	29.571	54.461	1.00	55.14	8
ATOM	1546	OE2	GLU	A	195	6.631	27.966	52.956	1.00	57.75	8
ATOM	1547	C	GLU	A	195	9.700	28.208	52.047	1.00	39.50	6
ATOM	1548	O	GLU	A	195	8.651	28.431	51.452	1.00	40.21	8
ATOM	1549	N	TYR	A	196	10.689	29.096	52.098	1.00	37.13	7
ATOM	1550	CA	TYR	A	196	10.549	30.379	51.434	1.00	35.50	6
ATOM	1551	CB	TYR	A	196	9.602	31.274	52.245	1.00	36.36	6
ATOM	1552	CG	TYR	A	196	10.175	31.816	53.538	1.00	37.28	6
ATOM	1553	CD1	TYR	A	196	11.120	32.848	53.527	1.00	35.42	6
ATOM	1554	CE1	TYR	A	196	11.637	33.366	54.706	1.00	33.10	6
ATOM	1555	CD2	TYR	A	196	9.764	31.311	54.776	1.00	36.75	6
ATOM	1556	CE2	TYR	A	196	10.279	31.825	55.968	1.00	35.26	6
ATOM	1557	CZ	TYR	A	196	11.213	32.856	55.922	1.00	35.84	6
ATOM	1558	OH	TYR	A	196	11.704	33.401	57.087	1.00	37.09	8
ATOM	1559	C	TYR	A	196	11.878	31.097	51.188	1.00	34.89	6
ATOM	1560	O	TYR	A	196	11.896	32.256	50.764	1.00	31.61	8
ATOM	1561	N	ALA	A	197	12.991	30.416	51.437	1.00	34.39	7
ATOM	1562	CA	ALA	A	197	14.297	31.041	51.242	1.00	34.82	6
ATOM	1563	CB	ALA	A	197	14.684	31.826	52.489	1.00	32.48	6
ATOM	1564	C	ALA	A	197	15.418	30.075	50.887	1.00	36.59	6
ATOM	1565	O	ALA	A	197	15.407	28.903	51.291	1.00	37.46	8
ATOM	1566	N	PHE	A	198	16.388	30.584	50.133	1.00	36.22	7
ATOM	1567	CA	PHE	A	198	17.548	29.802	49.722	1.00	37.68	6
ATOM	1568	CB	PHE	A	198	18.597	30.729	49.109	1.00	40.89	6
ATOM	1569	CG	PHE	A	198	19.810	30.013	48.578	1.00	43.59	6
ATOM	1570	CD1	PHE	A	198	19.783	29.404	47.325	1.00	44.74	6
ATOM	1571	CD2	PHE	A	198	20.970	29.929	49.336	1.00	41.86	6
ATOM	1572	CE1	PHE	A	198	20.894	28.729	46.833	1.00	41.42	6
ATOM	1573	CE2	PHE	A	198	22.079	29.251	48.849	1.00	43.30	6
ATOM	1574	CZ	PHE	A	198	22.040	28.652	47.595	1.00	41.86	6
ATOM	1575	C	PHE	A	198	18.139	29.140	50.967	1.00	37.00	6
ATOM	1576	O	PHE	A	198	18.166	29.754	52.036	1.00	36.43	8
ATOM	1577	N	PRO	A	199	18.641	27.892	50.848	1.00	37.63	7
ATOM	1578	CD	PRO	A	199	19.298	27.238	51.997	1.00	35.29	6
ATOM	1579	CA	PRO	A	199	18.727	27.008	49.673	1.00	36.52	6
ATOM	1580	CB	PRO	A	199	19.702	25.936	50.138	1.00	34.96	6
ATOM	1581	CG	PRO	A	199	19.281	25.770	51.565	1.00	34.57	6
ATOM	1582	C	PRO	A	199	17.409	26.380	49.222	1.00	35.72	6
ATOM	1583	O	PRO	A	199	17.386	25.663	48.225	1.00	37.36	8
ATOM	1584	N	PHE	A	200	16.331	26.638	49.962	1.00	33.78	7

92/263 Figure 17-25

ATOM	1585	CA	PHE	A	200	15.004	26.090	49.662	1.00	32.15	6
ATOM	1586	CB	PHE	A	200	14.562	26.381	48.222	1.00	28.39	6
ATOM	1587	CG	PHE	A	200	14.600	27.827	47.835	1.00	26.29	6
ATOM	1588	CD1	PHE	A	200	15.749	28.385	47.296	1.00	24.82	6
ATOM	1589	CD2	PHE	A	200	13.466	28.623	47.966	1.00	28.04	6
ATOM	1590	CE1	PHE	A	200	15.767	29.712	46.882	1.00	25.68	6
ATOM	1591	CE2	PHE	A	200	13.475	29.955	47.557	1.00	27.03	6
ATOM	1592	CZ	PHE	A	200	14.626	30.498	47.013	1.00	24.90	6
ATOM	1593	C	PHE	A	200	14.947	24.574	49.842	1.00	32.66	6
ATOM	1594	O	PHE	A	200	13.925	24.033	50.264	1.00	31.22	8
ATOM	1595	N	GLU	A	201	16.043	23.896	49.499	1.00	33.60	7
ATOM	1596	CA	GLU	A	201	16.128	22.438	49.585	1.00	30.86	6
ATOM	1597	CB	GLU	A	201	17.213	21.931	48.637	1.00	32.98	6
ATOM	1598	CG	GLU	A	201	16.879	22.182	47.175	1.00	33.52	6
ATOM	1599	CD	GLU	A	201	18.012	21.864	46.232	1.00	34.56	6
ATOM	1600	OE1	GLU	A	201	18.396	20.678	46.117	1.00	36.35	8
ATOM	1601	OE2	GLU	A	201	18.523	22.814	45.605	1.00	36.52	8
ATOM	1602	C	GLU	A	201	16.369	21.911	50.981	1.00	28.52	6
ATOM	1603	O	GLU	A	201	15.537	21.199	51.520	1.00	28.91	8
ATOM	1604	N	LYS	A	202	17.511	22.239	51.566	1.00	31.64	7
ATOM	1605	CA	LYS	A	202	17.795	21.780	52.917	1.00	32.34	6
ATOM	1606	CB	LYS	A	202	19.276	21.432	53.092	1.00	36.91	6
ATOM	1607	CG	LYS	A	202	19.789	20.226	52.307	1.00	43.74	6
ATOM	1608	CD	LYS	A	202	20.212	20.590	50.891	1.00	49.31	6
ATOM	1609	CE	LYS	A	202	20.952	19.428	50.227	1.00	49.34	6
ATOM	1610	NZ	LYS	A	202	21.504	19.802	48.895	1.00	49.89	7
ATOM	1611	C	LYS	A	202	17.421	22.849	53.937	1.00	30.55	6
ATOM	1612	O	LYS	A	202	16.877	23.890	53.586	1.00	26.55	8
ATOM	1613	N	GLY	A	203	17.710	22.571	55.203	1.00	30.59	7
ATOM	1614	CA	GLY	A	203	17.422	23.519	56.259	1.00	30.24	6
ATOM	1615	C	GLY	A	203	16.216	23.210	57.125	1.00	29.23	6
ATOM	1616	O	GLY	A	203	15.915	23.975	58.041	1.00	32.90	8
ATOM	1617	N	PHE	A	204	15.526	22.104	56.866	1.00	26.32	7
ATOM	1618	CA	PHE	A	204	14.344	21.779	57.657	1.00	23.25	6
ATOM	1619	CB	PHE	A	204	13.366	20.917	56.863	1.00	21.25	6
ATOM	1620	CG	PHE	A	204	12.855	21.573	55.635	1.00	18.60	6
ATOM	1621	CD1	PHE	A	204	13.605	21.560	54.461	1.00	16.43	6
ATOM	1622	CD2	PHE	A	204	11.654	22.273	55.664	1.00	14.82	6
ATOM	1623	CE1	PHE	A	204	13.168	22.245	53.333	1.00	16.91	6
ATOM	1624	CE2	PHE	A	204	11.206	22.962	54.544	1.00	15.28	6
ATOM	1625	CZ	PHE	A	204	11.965	22.952	53.375	1.00	18.34	6
ATOM	1626	C	PHE	A	204	14.626	21.094	58.979	1.00	23.72	6
ATOM	1627	O	PHE	A	204	15.578	20.318	59.118	1.00	22.68	8
ATOM	1628	N	LEU	A	205	13.760	21.376	59.942	1.00	20.94	7
ATOM	1629	CA	LEU	A	205	13.877	20.818	61.272	1.00	24.83	6
ATOM	1630	CB	LEU	A	205	12.678	21.259	62.110	1.00	21.29	6
ATOM	1631	CG	LEU	A	205	12.672	20.811	63.568	1.00	22.67	6
ATOM	1632	CD1	LEU	A	205	14.011	21.182	74.245	1.00	19.76	6
ATOM	1633	CD2	LEU	A	205	11.478	21.456	64.275	1.00	20.62	6
ATOM	1634	C	LEU	A	205	14.002	19.293	61.303	1.00	28.79	6
ATOM	1635	O	LEU	A	205	14.443	18.730	62.310	1.00	28.59	8
ATOM	1636	N	GLU	A	206	13.625	18.628	60.211	1.00	33.52	7
ATOM	1637	CA	GLU	A	206	13.693	17.166	60.142	1.00	39.79	6
ATOM	1638	CB	GLU	A	206	12.736	16.616	59.070	1.00	44.37	6
ATOM	1639	CG	GLU	A	206	11.284	17.060	59.204	1.00	50.75	6
ATOM	1640	CD	GLU	A	206	11.014	18.390	58.512	1.00	55.31	6
ATOM	1641	OE1	GLU	A	206	9.972	19.027	58.797	1.00	55.36	8
ATOM	1642	OE2	GLU	A	206	11.839	18.786	57.661	1.00	56.48	8
ATOM	1643	C	GLU	A	206	15.114	16.674	59.847	1.00	40.00	6
ATOM	1644	O	GLU	A	206	15.483	15.541	60.180	1.00	39.35	8
ATOM	1645	N	GLU	A	207	15.903	17.536	59.217	1.00	39.38	7
ATOM	1646	CA	GLU	A	207	17.286	17.219	58.873	1.00	37.90	6
ATOM	1647	CB	GLU	A	207	17.776	18.242	57.854	1.00	37.36	6
ATOM	1648	CG	GLU	A	207	16.983	18.158	56.556	1.00	37.29	6
ATOM	1649	CD	GLU	A	207	16.978	19.452	55.773	1.00	38.16	6
ATOM	1650	OE1	GLU	A	207	18.071	20.016	55.537	1.00	35.44	8

ATOM	1651	OE2	GLU A 207	15.870	19.891	55.389	1.00	34.62	8
ATOM	1652	C	GLU A 207	18.139	17.239	60.134	1.00	36.18	6
ATOM	1653	O	GLU A 207	18.560	18.303	60.590	1.00	34.81	8
ATOM	1654	N	ILE A 208	18.381	16.059	60.701	1.00	34.45	7
ATOM	1655	CA	ILE A 208	19.164	15.965	61.932	1.00	38.53	6
ATOM	1656	CB	ILE A 208	18.260	15.511	63.117	1.00	41.12	6
ATOM	1657	CG2	ILE A 208	19.097	15.273	64.375	1.00	41.36	6
ATOM	1658	CG1	ILE A 208	17.193	16.581	63.383	1.00	42.21	6
ATOM	1659	CD1	ILE A 208	16.291	16.286	64.560	1.00	44.81	6
ATOM	1660	C	ILE A 208	20.407	15.074	61.876	1.00	36.66	6
ATOM	1661	O	ILE A 208	21.243	15.110	62.775	1.00	34.03	8
ATOM	1662	N	GLY A 209	20.540	14.284	60.822	1.00	36.80	7
ATOM	1663	CA	GLY A 209	21.703	13.428	60.728	1.00	38.99	6
ATOM	1664	C	GLY A 209	21.509	12.246	59.805	1.00	40.93	6
ATOM	1665	O	GLY A 209	20.477	12.124	59.145	1.00	40.26	8
ATOM	1666	N	GLU A 210	22.508	11.370	59.775	1.00	42.16	7
ATOM	1667	CA	GLU A 210	22.492	10.185	58.930	1.00	43.30	6
ATOM	1668	CB	GLU A 210	22.810	10.586	57.488	1.00	47.08	6
ATOM	1669	CG	GLU A 210	22.826	9.453	56.478	1.00	53.90	6
ATOM	1670	CD	GLU A 210	23.256	9.915	55.089	1.00	56.27	6
ATOM	1671	OE1	GLU A 210	24.412	10.371	54.941	1.00	56.19	8
ATOM	1672	OE2	GLU A 210	22.437	9.826	54.145	1.00	60.28	8
ATOM	1673	C	GLU A 210	23.583	9.276	59.473	1.00	41.47	6
ATOM	1674	O	GLU A 210	24.750	9.457	59.152	1.00	43.97	8
ATOM	1675	N	GLY A 211	23.203	8.307	60.299	1.00	39.97	7
ATOM	1676	CA	GLY A 211	24.181	7.405	60.885	1.00	37.34	6
ATOM	1677	C	GLY A 211	24.642	7.952	62.224	1.00	37.84	6
ATOM	1678	O	GLY A 211	23.820	8.408	63.019	1.00	37.30	8
ATOM	1679	N	LYS A 212	25.948	7.910	62.485	1.00	38.52	7
ATOM	1680	CA	LYS A 212	26.490	8.440	63.733	1.00	38.29	6
ATOM	1681	CB	LYS A 212	28.020	8.359	63.731	1.00	40.54	6
ATOM	1682	CG	LYS A 212	28.570	6.950	63.675	1.00	46.39	6
ATOM	1683	CD	LYS A 212	28.149	6.147	64.910	1.00	51.59	6
ATOM	1684	CE	LYS A 212	28.556	4.676	64.809	1.00	52.77	6
ATOM	1685	NZ	LYS A 212	30.030	4.478	64.662	1.00	55.48	7
ATOM	1686	C	LYS A 212	26.061	9.897	63.866	1.00	37.68	6
ATOM	1687	O	LYS A 212	25.814	10.389	64.962	1.00	34.75	8
ATOM	1688	N	GLY A 213	25.956	10.574	62.728	1.00	38.89	7
ATOM	1689	CA	GLY A 213	25.577	11.975	62.724	1.00	43.58	6
ATOM	1690	C	GLY A 213	24.126	12.295	63.020	1.00	43.99	6
ATOM	1691	O	GLY A 213	23.737	13.464	63.024	1.00	44.67	8
ATOM	1692	N	LYS A 214	23.321	11.268	63.265	1.00	46.02	7
ATOM	1693	CA	LYS A 214	21.907	11.467	63.562	1.00	45.61	6
ATOM	1694	CB	LYS A 214	21.168	10.130	63.469	1.00	47.77	6
ATOM	1695	CG	LYS A 214	19.675	10.252	63.249	1.00	49.25	6
ATOM	1696	CD	LYS A 214	19.078	8.901	62.911	1.00	51.64	6
ATOM	1697	CE	LYS A 214	17.637	9.038	62.440	1.00	54.30	6
ATOM	1698	NZ	LYS A 214	17.030	7.727	62.034	1.00	56.09	7
ATOM	1699	C	LYS A 214	21.809	12.047	64.970	1.00	44.22	6
ATOM	1700	O	LYS A 214	22.210	11.410	65.942	1.00	45.04	8
ATOM	1701	N	GLY A 215	21.292	13.266	65.074	1.00	42.89	7
ATOM	1702	CA	GLY A 215	21.193	13.904	66.373	1.00	40.20	6
ATOM	1703	C	GLY A 215	22.295	14.931	66.600	1.00	39.90	6
ATOM	1704	O	GLY A 215	22.356	15.548	67.668	1.00	40.12	8
ATOM	1705	N	TYR A 216	23.175	15.111	65.612	1.00	38.49	7
ATOM	1706	CA	TYR A 216	24.261	16.086	65.726	1.00	35.91	6
ATOM	1707	CB	TYR A 216	25.632	15.421	65.618	1.00	36.47	6
ATOM	1708	CG	TYR A 216	25.935	14.461	66.738	1.00	39.54	6
ATOM	1709	CD1	TYR A 216	25.296	13.220	66.810	1.00	40.62	6
ATOM	1710	CE1	TYR A 216	25.561	12.333	67.849	1.00	41.58	6
ATOM	1711	CD2	TYR A 216	26.852	14.795	67.739	1.00	39.20	6
ATOM	1712	CE2	TYR A 216	27.124	13.915	68.786	1.00	40.87	6
ATOM	1713	CZ	TYR A 216	26.475	12.685	68.833	1.00	41.86	6
ATOM	1714	OH	TYR A 216	26.743	11.802	69.852	1.00	43.04	8
ATOM	1715	C	TYR A 216	24.182	17.215	64.709	1.00	34.21	6
ATOM	1716	O	TYR A 216	25.194	17.832	64.375	1.00	33.37	8

ATOM	1717	N	ASN	A	217	22.976	17.471	64.212	1.00	33.83	7
ATOM	1718	CA	ASN	A	217	22.726	18.558	63.267	1.00	30.20	6
ATOM	1719	CB	ASN	A	217	22.699	18.057	61.823	1.00	27.74	6
ATOM	1720	CG	ASN	A	217	22.457	19.177	60.826	1.00	25.61	6
ATOM	1721	OD1	ASN	A	217	21.354	19.705	60.719	1.00	25.00	8
ATOM	1722	ND2	ASN	A	217	23.501	19.558	60.103	1.00	30.43	7
ATOM	1723	C	ASN	A	217	21.369	19.116	63.645	1.00	29.09	6
ATOM	1724	O	ASN	A	217	20.433	18.351	63.885	1.00	26.93	8
ATOM	1725	N	LEU	A	218	21.263	20.440	63.710	1.00	27.19	7
ATOM	1726	CA	LEU	A	218	20.010	21.071	64.089	1.00	25.33	6
ATOM	1727	CB	LEU	A	218	20.026	21.379	65.590	1.00	23.23	6
ATOM	1728	CG	LEU	A	218	18.729	21.704	66.346	1.00	21.00	6
ATOM	1729	CD1	LEU	A	218	19.100	22.313	67.695	1.00	18.62	6
ATOM	1730	CD2	LEU	A	218	17.872	22.675	65.583	1.00	18.48	6
ATOM	1731	C	LEU	A	218	19.785	22.368	63.325	1.00	25.04	6
ATOM	1732	O	LEU	A	218	20.596	23.287	63.415	1.00	25.23	8
ATOM	1733	N	ASN	A	219	18.681	22.436	62.584	1.00	28.44	7
ATOM	1734	CA	ASN	A	219	18.310	23.636	61.829	1.00	28.76	6
ATOM	1735	CB	ASN	A	219	17.809	23.298	60.417	1.00	25.69	6
ATOM	1736	CG	ASN	A	219	18.748	22.408	59.646	1.00	26.10	6
ATOM	1737	OD1	ASN	A	219	19.927	22.708	59.505	1.00	28.53	8
ATOM	1738	ND2	ASN	A	219	18.220	21.311	59.114	1.00	26.97	7
ATOM	1739	C	ASN	A	219	17.129	24.248	62.582	1.00	31.96	6
ATOM	1740	O	ASN	A	219	16.373	23.539	63.246	1.00	34.84	8
ATOM	1741	N	ILE	A	220	16.952	25.556	62.472	1.00	32.96	7
ATOM	1742	CA	ILE	A	220	15.826	26.196	63.129	1.00	32.50	6
ATOM	1743	CB	ILE	A	220	16.259	27.037	64.350	1.00	32.32	6
ATOM	1744	CG2	ILE	A	220	15.029	27.644	65.014	1.00	29.46	6
ATOM	1745	CG1	ILE	A	220	16.978	26.160	65.374	1.00	29.65	6
ATOM	1746	CD1	ILE	A	220	16.080	25.138	66.027	1.00	28.65	6
ATOM	1747	C	ILE	A	220	15.140	27.106	62.123	1.00	35.36	6
ATOM	1748	O	ILE	A	220	15.469	28.290	62.009	1.00	35.52	8
ATOM	1749	N	PRO	A	221	14.185	26.553	61.359	1.00	36.87	7
ATOM	1750	CD	PRO	A	221	13.718	25.158	61.359	1.00	35.12	6
ATOM	1751	CA	PRO	A	221	13.445	27.318	60.356	1.00	35.41	6
ATOM	1752	CB	PRO	A	221	12.509	26.262	59.767	1.00	35.68	6
ATOM	1753	CG	PRO	A	221	13.319	24.992	59.911	1.00	33.86	6
ATOM	1754	C	PRO	A	221	12.696	28.437	61.053	1.00	34.37	6
ATOM	1755	O	PRO	A	221	12.014	28.199	62.043	1.00	38.79	8
ATOM	1756	N	LEU	A	222	12.815	29.655	60.547	1.00	34.76	7
ATOM	1757	CA	LEU	A	222	12.138	30.796	61.166	1.00	33.87	6
ATOM	1758	CB	LEU	A	222	13.173	31.735	61.798	1.00	35.13	6
ATOM	1759	CG	LEU	A	222	14.104	31.163	62.876	1.00	33.07	6
ATOM	1760	CD1	LEU	A	222	15.234	32.150	63.154	1.00	34.04	6
ATOM	1761	CD2	LEU	A	222	13.312	30.856	64.141	1.00	32.39	6
ATOM	1762	C	LEU	A	222	11.287	31.567	60.157	1.00	32.15	6
ATOM	1763	O	LEU	A	222	11.669	31.740	59.000	1.00	31.32	8
ATOM	1764	N	PRO	A	223	10.127	32.060	60.601	1.00	30.97	7
ATOM	1765	CD	PRO	A	223	9.606	31.913	61.972	1.00	32.34	6
ATOM	1766	CA	PRO	A	223	9.173	32.818	59.789	1.00	30.55	6
ATOM	1767	CB	PRO	A	223	7.957	32.893	60.702	1.00	29.44	6
ATOM	1768	CG	PRO	A	223	8.626	33.068	62.046	1.00	31.02	6
ATOM	1769	C	PRO	A	223	9.645	34.205	59.366	1.00	29.20	6
ATOM	1770	O	PRO	A	223	10.694	34.680	59.796	1.00	31.95	8
ATOM	1771	N	LYS	A	224	8.841	34.841	58.521	1.00	26.14	7
ATOM	1772	CA	LYS	A	224	9.115	36.172	58.026	1.00	23.54	6
ATOM	1773	CB	LYS	A	224	8.285	36.443	56.766	1.00	24.71	6
ATOM	1774	CG	LYS	A	224	8.563	35.500	55.619	1.00	23.83	6
ATOM	1775	CD	LYS	A	224	7.737	35.800	54.394	1.00	20.59	6
ATOM	1776	CE	LYS	A	224	8.065	34.769	53.329	1.00	27.03	6
ATOM	1777	NZ	LYS	A	224	7.198	34.849	52.122	1.00	30.48	7
ATOM	1778	C	LYS	A	224	8.702	37.151	59.111	1.00	25.48	6
ATOM	1779	O	LYS	A	224	7.999	36.780	60.055	1.00	22.67	8
ATOM	1780	N	GLY	A	225	9.124	38.404	58.960	1.00	26.88	7
ATOM	1781	CA	GLY	A	225	8.777	39.432	59.925	1.00	29.80	6
ATOM	1782	C	GLY	A	225	9.396	39.188	61.286	1.00	32.96	6

95/263 Figure 17-28

ATOM	1783	O	GLY	A	225	9.068	39.861	62.271	1.00	31.20	8
ATOM	1784	N	LEU	A	226	10.299	38.216	61.338	1.00	32.86	7
ATOM	1785	CA	LEU	A	226	10.975	37.877	62.575	1.00	34.55	6
ATOM	1786	CB	LEU	A	226	12.149	36.958	62.255	1.00	34.46	6
ATOM	1787	CG	LEU	A	226	12.982	36.413	63.407	1.00	34.48	6
ATOM	1788	CD1	LEU	A	226	12.146	35.425	64.212	1.00	33.18	6
ATOM	1789	CD2	LEU	A	226	14.207	35.724	62.847	1.00	31.39	6
ATOM	1790	C	LEU	A	226	11.481	39.160	63.255	1.00	36.29	6
ATOM	1791	O	LEU	A	226	12.156	39.970	62.613	1.00	33.87	8
ATOM	1792	N	ASN	A	227	11.131	39.358	64.531	1.00	37.31	7
ATOM	1793	CA	ASN	A	227	11.592	40.536	65.279	1.00	37.26	6
ATOM	1794	CB	ASN	A	227	10.444	41.212	66.053	1.00	35.57	6
ATOM	1795	CG	ASN	A	227	9.920	40.368	67.208	1.00	36.07	6
ATOM	1796	OD1	ASN	A	227	10.678	39.940	68.089	1.00	35.08	8
ATOM	1797	ND2	ASN	A	227	8.611	40.143	67.218	1.00	32.33	7
ATOM	1798	C	ASN	A	227	12.688	40.096	66.250	1.00	37.95	6
ATOM	1799	O	ASN	A	227	12.869	38.890	66.473	1.00	37.08	8
ATOM	1800	N	ASP	A	228	13.403	41.063	66.832	1.00	36.07	7
ATOM	1801	CA	ASP	A	228	14.505	40.754	67.751	1.00	37.63	6
ATOM	1802	CB	ASP	A	228	14.996	42.007	68.486	1.00	36.48	6
ATOM	1803	CG	ASP	A	228	15.480	43.088	67.545	1.00	37.52	6
ATOM	1804	OD1	ASP	A	228	15.936	42.752	66.427	1.00	35.28	8
ATOM	1805	OD2	ASP	A	228	15.426	44.274	67.937	1.00	39.01	8
ATOM	1806	C	ASP	A	228	14.204	39.678	68.783	1.00	37.56	6
ATOM	1807	O	ASP	A	228	14.921	38.678	68.869	1.00	39.53	8
ATOM	1808	N	ASN	A	229	13.155	39.889	69.572	1.00	38.37	7
ATOM	1809	CA	ASN	A	229	12.766	38.935	70.605	1.00	37.49	6
ATOM	1810	CB	ASN	A	229	11.422	39.352	71.200	1.00	37.38	6
ATOM	1811	CG	ASN	A	229	11.490	40.709	71.877	1.00	40.47	6
ATOM	1812	OD1	ASN	A	229	12.041	40.840	72.973	1.00	41.76	8
ATOM	1813	ND2	ASN	A	229	10.960	41.735	71.212	1.00	36.50	7
ATOM	1814	C	ASN	A	229	12.680	37.530	70.017	1.00	37.64	6
ATOM	1815	O	ASN	A	229	13.446	36.634	70.395	1.00	35.76	8
ATOM	1816	N	GLU	A	230	11.758	37.351	69.076	1.00	36.01	7
ATOM	1817	CA	GLU	A	230	11.574	36.062	68.425	1.00	34.74	6
ATOM	1818	CB	GLU	A	230	10.753	36.242	67.153	1.00	35.55	6
ATOM	1819	CG	GLU	A	230	9.382	36.820	67.407	1.00	36.95	6
ATOM	1820	CD	GLU	A	230	8.580	36.960	66.144	1.00	35.30	6
ATOM	1821	OE1	GLU	A	230	9.042	37.670	65.229	1.00	36.98	8
ATOM	1822	OE2	GLU	A	230	7.490	36.361	66.065	1.00	36.71	8
ATOM	1823	C	GLU	A	230	12.916	35.421	68.082	1.00	33.92	6
ATOM	1824	O	GLU	A	230	13.143	34.238	68.346	1.00	32.74	8
ATOM	1825	N	PHE	A	231	13.804	36.207	67.487	1.00	32.03	7
ATOM	1826	CA	PHE	A	231	15.116	35.712	67.123	1.00	30.55	6
ATOM	1827	CB	PHE	A	231	15.932	36.821	66.460	1.00	33.86	6
ATOM	1828	CG	PHE	A	231	17.295	36.381	66.012	1.00	36.97	6
ATOM	1829	CD1	PHE	A	231	17.438	35.334	65.102	1.00	40.41	6
ATOM	1830	CD2	PHE	A	231	18.436	37.021	66.480	1.00	36.58	6
ATOM	1831	CE1	PHE	A	231	18.709	34.932	64.661	1.00	43.00	6
ATOM	1832	CE2	PHE	A	231	19.711	36.632	66.049	1.00	39.07	6
ATOM	1833	CZ	PHE	A	231	19.849	35.586	65.137	1.00	40.52	6
ATOM	1834	C	PHE	A	231	15.835	35.232	68.376	1.00	30.63	6
ATOM	1835	O	PHE	A	231	16.177	34.042	68.497	1.00	29.66	8
ATOM	1836	N	LEU	A	232	16.049	36.162	69.310	1.00	24.94	7
ATOM	1837	CA	LEU	A	232	16.742	35.857	70.556	1.00	22.82	6
ATOM	1838	CB	LEU	A	232	16.724	37.084	71.468	1.00	24.96	6
ATOM	1839	CG	LEU	A	232	17.507	38.282	70.890	1.00	29.34	6
ATOM	1840	CD1	LEU	A	232	17.316	39.549	71.746	1.00	24.38	6
ATOM	1841	CD2	LEU	A	232	18.991	37.903	70.787	1.00	27.39	6
ATOM	1842	C	LEU	A	232	16.150	34.638	71.261	1.00	22.44	6
ATOM	1843	O	LEU	A	232	16.882	33.793	71.767	1.00	20.37	8
ATOM	1844	N	PHE	A	233	14.825	34.552	71.289	1.00	24.81	7
ATOM	1845	CA	PHE	A	233	14.131	33.422	71.905	1.00	25.81	6
ATOM	1846	CB	PHE	A	233	12.623	33.535	71.641	1.00	24.37	6
ATOM	1847	CG	PHE	A	233	11.811	32.373	72.157	1.00	24.18	6
ATOM	1848	CD1	PHE	A	233	11.491	32.264	73.503	1.00	25.59	6

ATOM	1849	CD2	PHE	A	233	11.339	31.397	71.284	1.00	25.75	6
ATOM	1850	CE1	PHE	A	233	10.698	31.198	73.974	1.00	25.33	6
ATOM	1851	CE2	PHE	A	233	10.548	30.327	71.747	1.00	24.02	6
ATOM	1852	CZ	PHE	A	233	10.228	30.232	73.093	1.00	22.77	6
ATOM	1853	C	PHE	A	233	14.661	32.133	71.275	1.00	26.64	6
ATOM	1854	O	PHE	A	233	15.094	31.209	71.971	1.00	28.34	8
ATOM	1855	N	ALA	A	234	14.624	32.087	69.949	1.00	27.27	7
ATOM	1856	CA	ALA	A	234	15.080	30.921	69.209	1.00	30.24	6
ATOM	1857	CB	ALA	A	234	14.797	31.107	67.720	1.00	33.38	6
ATOM	1858	C	ALA	A	234	16.563	30.645	69.433	1.00	30.76	6
ATOM	1859	O	ALA	A	234	16.981	29.491	69.488	1.00	30.04	8
ATOM	1860	N	LEU	A	235	17.363	31.695	69.563	1.00	31.84	7
ATOM	1861	CA	LEU	A	235	18.789	31.486	69.790	1.00	32.83	6
ATOM	1862	CB	LEU	A	235	19.548	32.819	69.703	1.00	34.12	6
ATOM	1863	CG	LEU	A	235	21.039	32.745	69.316	1.00	36.33	6
ATOM	1864	CD1	LEU	A	235	21.625	34.156	69.205	1.00	36.44	6
ATOM	1865	CD2	LEU	A	235	21.803	31.939	70.330	1.00	35.64	6
ATOM	1866	C	LEU	A	235	18.970	30.846	71.176	1.00	30.75	6
ATOM	1867	O	LEU	A	235	19.648	29.835	71.312	1.00	30.12	8
ATOM	1868	N	GLU	A	236	18.347	31.435	72.192	1.00	29.03	7
ATOM	1869	CA	GLU	A	236	18.418	30.931	73.561	1.00	33.32	6
ATOM	1870	CB	GLU	A	236	17.479	31.730	74.452	1.00	35.06	6
ATOM	1871	CG	GLU	A	236	17.843	33.176	74.635	1.00	42.35	6
ATOM	1872	CD	GLU	A	236	16.610	34.022	74.843	1.00	47.12	6
ATOM	1873	OE1	GLU	A	236	15.686	33.557	75.556	1.00	48.91	8
ATOM	1874	OE2	GLU	A	236	16.572	35.150	74.297	1.00	49.07	8
ATOM	1875	C	GLU	A	236	17.988	29.473	73.639	1.00	34.65	6
ATOM	1876	O	GLU	A	236	18.715	28.593	74.116	1.00	30.43	8
ATOM	1877	N	LYS	A	237	16.767	29.250	73.176	1.00	35.67	7
ATOM	1878	CA	LYS	A	237	16.138	27.943	73.175	1.00	35.51	6
ATOM	1879	CB	LYS	A	237	14.791	28.060	72.452	1.00	37.01	6
ATOM	1880	CG	LYS	A	237	13.745	27.032	72.848	1.00	39.65	6
ATOM	1881	CD	LYS	A	237	12.712	27.605	73.821	1.00	40.66	6
ATOM	1882	CE	LYS	A	237	13.312	28.054	75.153	1.00	40.58	6
ATOM	1883	NZ	LYS	A	237	12.250	28.556	76.083	1.00	32.05	7
ATOM	1884	C	LYS	A	237	17.025	26.891	72.485	1.00	35.07	6
ATOM	1885	O	LYS	A	237	17.315	25.833	73.061	1.00	30.60	8
ATOM	1886	N	SER	A	238	17.455	27.200	71.259	1.00	33.59	7
ATOM	1887	CA	SER	A	238	18.279	26.293	70.452	1.00	32.18	6
ATOM	1888	CB	SER	A	238	18.453	26.867	69.042	1.00	32.01	6
ATOM	1889	OG	SER	A	238	19.014	28.168	69.075	1.00	37.80	8
ATOM	1890	C	SER	A	238	19.650	25.928	71.032	1.00	31.94	6
ATOM	1891	O	SER	A	238	20.064	24.758	70.990	1.00	26.88	8
ATOM	1892	N	LEU	A	239	20.357	26.920	71.564	1.00	31.19	7
ATOM	1893	CA	LEU	A	239	21.660	26.650	72.147	1.00	30.82	6
ATOM	1894	CB	LEU	A	239	22.293	27.914	72.720	1.00	28.03	6
ATOM	1895	CG	LEU	A	239	22.650	29.087	71.817	1.00	24.31	6
ATOM	1896	CD1	LEU	A	239	23.210	30.189	72.695	1.00	24.63	6
ATOM	1897	CD2	LEU	A	239	23.663	28.681	70.770	1.00	23.11	6
ATOM	1898	C	LEU	A	239	21.463	25.666	73.275	1.00	31.99	6
ATOM	1899	O	LEU	A	239	22.279	24.764	73.473	1.00	32.57	8
ATOM	1900	N	GLU	A	240	20.367	25.835	74.009	1.00	33.86	7
ATOM	1901	CA	GLU	A	240	20.094	24.965	75.136	1.00	38.61	6
ATOM	1902	CB	GLU	A	240	18.799	25.369	75.842	1.00	43.21	6
ATOM	1903	CG	GLU	A	240	18.500	24.468	77.045	1.00	53.52	6
ATOM	1904	CD	GLU	A	240	19.677	24.383	78.022	1.00	56.39	6
ATOM	1905	OE1	GLU	A	240	19.969	25.399	78.701	1.00	57.81	8
ATOM	1906	OE2	GLU	A	240	20.318	23.304	78.093	1.00	55.12	8
ATOM	1907	C	GLU	A	240	20.033	23.507	74.722	1.00	39.28	6
ATOM	1908	O	GLU	A	240	20.532	22.630	75.437	1.00	38.83	8
ATOM	1909	N	ILE	A	241	19.423	23.252	73.567	1.00	40.74	7
ATOM	1910	CA	ILE	A	241	19.310	21.896	73.035	1.00	38.08	6
ATOM	1911	CB	ILE	A	241	18.465	21.871	71.734	1.00	33.57	6
ATOM	1912	CG2	ILE	A	241	18.536	20.506	71.086	1.00	31.39	6
ATOM	1913	CG1	ILE	A	241	17.012	22.226	72.056	1.00	31.06	6
ATOM	1914	CD1	ILE	A	241	16.147	22.478	70.843	1.00	27.53	6

Figure 17-30

ATOM	1915	C	ILE	A	241	20.713	21.372	72.747	1.00	39.56	6
ATOM	1916	O	ILE	A	241	20.984	20.189	72.936	1.00	40.82	8
ATOM	1917	N	VAL	A	242	21.605	22.254	72.299	1.00	41.93	7
ATOM	1918	CA	VAL	A	242	22.979	21.842	72.015	1.00	45.09	6
ATOM	1919	CB	VAL	A	242	23.808	22.959	71.329	1.00	45.76	6
ATOM	1920	CG1	VAL	A	242	25.242	22.479	71.116	1.00	43.09	6
ATOM	1921	CG2	VAL	A	242	23.182	23.334	69.991	1.00	46.41	6
ATOM	1922	C	VAL	A	242	23.698	21.453	73.300	1.00	45.69	6
ATOM	1923	O	VAL	A	242	24.191	20.331	73.423	1.00	46.30	8
ATOM	1924	N	LYS	A	243	23.750	22.373	74.259	1.00	44.60	7
ATOM	1925	CA	LYS	A	243	24.427	22.088	75.513	1.00	46.96	6
ATOM	1926	CB	LYS	A	243	24.214	23.217	76.527	1.00	49.49	6
ATOM	1927	CG	LYS	A	243	25.061	23.023	77.795	1.00	54.90	6
ATOM	1928	CD	LYS	A	243	24.652	23.934	78.939	1.00	58.95	6
ATOM	1929	CE	LYS	A	243	24.782	25.399	78.577	1.00	64.13	6
ATOM	1930	NZ	LYS	A	243	24.274	26.283	79.676	1.00	66.93	7
ATOM	1931	C	LYS	A	243	23.965	20.767	76.135	1.00	47.06	6
ATOM	1932	O	LYS	A	243	24.735	20.113	76.845	1.00	46.39	8
ATOM	1933	N	GLU	A	244	22.716	20.380	75.878	1.00	47.51	7
ATOM	1934	CA	GLU	A	244	22.172	19.136	76.429	1.00	51.33	6
ATOM	1935	CB	GLU	A	244	20.650	19.061	76.259	1.00	54.49	6
ATOM	1936	CG	GLU	A	244	19.843	20.199	76.842	1.00	62.61	6
ATOM	1937	CD	GLU	A	244	18.360	20.089	76.489	1.00	65.15	6
ATOM	1938	OE1	GLU	A	244	17.572	20.980	76.888	1.00	66.49	8
ATOM	1939	OE2	GLU	A	244	17.986	19.108	75.807	1.00	64.82	8
ATOM	1940	C	GLU	A	244	22.745	17.936	75.698	1.00	50.17	6
ATOM	1941	O	GLU	A	244	22.866	16.846	76.259	1.00	51.54	8
ATOM	1942	N	VAL	A	245	23.104	18.148	74.441	1.00	47.70	7
ATOM	1943	CA	VAL	A	245	23.587	17.063	73.611	1.00	45.43	6
ATOM	1944	CB	VAL	A	245	22.704	16.980	72.336	1.00	48.47	6
ATOM	1945	CG1	VAL	A	245	23.082	15.765	71.499	1.00	51.87	6
ATOM	1946	CG2	VAL	A	245	21.226	16.934	72.731	1.00	45.65	6
ATOM	1947	C	VAL	A	245	25.056	17.070	73.185	1.00	43.01	6
ATOM	1948	O	VAL	A	245	25.620	16.005	72.946	1.00	39.28	8
ATOM	1949	N	PHE	A	246	25.682	18.245	73.109	1.00	40.53	7
ATOM	1950	CA	PHE	A	246	27.063	18.321	72.633	1.00	38.56	6
ATOM	1951	CB	PHE	A	246	27.023	18.700	71.154	1.00	36.85	6
ATOM	1952	CG	PHE	A	246	28.315	18.487	70.415	1.00	36.46	6
ATOM	1953	CD1	PHE	A	246	28.749	17.201	70.098	1.00	32.95	6
ATOM	1954	CD2	PHE	A	246	29.064	19.582	69.967	1.00	35.51	6
ATOM	1955	CE1	PHE	A	246	29.903	17.004	69.337	1.00	33.80	6
ATOM	1956	CE2	PHE	A	246	30.222	19.397	69.206	1.00	34.46	6
ATOM	1957	CZ	PHE	A	246	30.640	18.103	68.889	1.00	35.54	6
ATOM	1958	C	PHE	A	246	27.970	19.311	73.371	1.00	40.83	6
ATOM	1959	O	PHE	A	246	27.613	20.478	73.549	1.00	40.32	8
ATOM	1960	N	GLU	A	247	29.141	18.839	73.802	1.00	42.54	7
ATOM	1961	CA	GLU	A	247	30.128	19.695	74.467	1.00	43.93	6
ATOM	1962	CB	GLU	A	247	30.655	19.075	75.770	1.00	45.67	6
ATOM	1963	CG	GLU	A	247	29.763	19.243	77.005	1.00	51.63	6
ATOM	1964	CD	GLU	A	247	28.478	18.424	76.962	1.00	57.42	6
ATOM	1965	OE1	GLU	A	247	27.645	18.644	76.058	1.00	62.12	8
ATOM	1966	OE2	GLU	A	247	28.296	17.557	77.845	1.00	59.43	8
ATOM	1967	C	GLU	A	247	31.268	19.839	73.464	1.00	43.62	6
ATOM	1968	O	GLU	A	247	32.077	18.931	73.294	1.00	44.25	8
ATOM	1969	N	PRO	A	248	31.342	20.988	72.780	1.00	43.65	7
ATOM	1970	CD	PRO	A	248	30.439	22.143	72.863	1.00	42.73	6
ATOM	1971	CA	PRO	A	248	32.371	21.260	71.779	1.00	43.28	6
ATOM	1972	CB	PRO	A	248	31.802	22.480	71.042	1.00	43.03	6
ATOM	1973	CG	PRO	A	248	30.317	22.474	71.415	1.00	43.02	6
ATOM	1974	C	PRO	A	248	33.759	21.552	72.331	1.00	43.37	6
ATOM	1975	O	PRO	A	248	33.896	22.286	73.305	1.00	45.44	8
ATOM	1976	N	GLU	A	249	34.788	20.982	71.710	1.00	42.38	7
ATOM	1977	CA	GLU	A	249	36.151	21.263	72.136	1.00	41.56	6
ATOM	1978	CB	GLU	A	249	37.148	20.275	71.528	1.00	42.06	6
ATOM	1979	CG	GLU	A	249	36.935	18.816	71.887	1.00	44.28	6
ATOM	1980	CD	GLU	A	249	38.015	17.908	71.295	1.00	44.79	6

Figure 17-31

ATOM	1981	OE1	GLU	A	249	38.208	17.938	70.054	1.00	42.47	8
ATOM	1982	OE2	GLU	A	249	38.666	17.168	72.072	1.00	39.73	8
ATOM	1983	C	GLU	A	249	36.443	22.654	71.583	1.00	40.99	6
ATOM	1984	O	GLU	A	249	37.150	23.450	72.204	1.00	42.83	8
ATOM	1985	N	VAL	A	250	35.879	22.936	70.407	1.00	37.65	7
ATOM	1986	CA	VAL	A	250	36.059	24.221	69.728	1.00	34.87	6
ATOM	1987	CB	VAL	A	250	37.294	24.203	68.789	1.00	34.53	6
ATOM	1988	CG1	VAL	A	250	37.129	23.113	67.728	1.00	32.76	6
ATOM	1989	CG2	VAL	A	250	37.487	25.581	68.144	1.00	29.62	6
ATOM	1990	C	VAL	A	250	34.830	24.527	68.891	1.00	32.67	6
ATOM	1991	O	VAL	A	250	34.162	23.610	68.421	1.00	33.96	8
ATOM	1992	N	TYR	A	251	34.539	25.810	68.690	1.00	29.71	7
ATOM	1993	CA	TYR	A	251	33.368	26.183	67.916	1.00	27.07	6
ATOM	1994	CB	TYR	A	251	32.185	26.451	68.860	1.00	29.11	6
ATOM	1995	CG	TYR	A	251	32.080	27.872	69.406	1.00	31.46	6
ATOM	1996	CD1	TYR	A	251	31.553	28.903	68.622	1.00	31.14	6
ATOM	1997	CE1	TYR	A	251	31.439	30.196	69.106	1.00	31.66	6
ATOM	1998	CD2	TYR	A	251	32.494	28.181	70.696	1.00	30.20	6
ATOM	1999	CE2	TYR	A	251	32.384	29.477	71.193	1.00	33.89	6
ATOM	2000	CZ	TYR	A	251	31.854	30.482	70.391	1.00	34.75	6
ATOM	2001	OH	TYR	A	251	31.743	31.773	70.867	1.00	33.52	8
ATOM	2002	C	TYR	A	251	33.570	27.384	66.992	1.00	27.48	6
ATOM	2003	O	TYR	A	251	34.167	28.402	67.366	1.00	24.78	8
ATOM	2004	N	LEU	A	252	33.063	27.254	65.773	1.00	24.80	7
ATOM	2005	CA	LEU	A	252	33.150	28.332	64.815	1.00	23.40	6
ATOM	2006	CB	LEU	A	252	33.631	27.810	63.451	1.00	21.32	6
ATOM	2007	CG	LEU	A	252	35.126	27.456	63.385	1.00	21.84	6
ATOM	2008	CD1	LEU	A	252	35.457	26.373	64.395	1.00	22.51	6
ATOM	2009	CD2	LEU	A	252	35.499	26.999	61.986	1.00	22.07	6
ATOM	2010	C	LEU	A	252	31.762	28.959	64.729	1.00	22.56	6
ATOM	2011	O	LEU	A	252	30.750	28.266	64.856	1.00	21.99	8
ATOM	2012	N	LEU	A	253	31.734	30.277	64.554	1.00	21.01	7
ATOM	2013	CA	LEU	A	253	30.498	31.047	64.461	1.00	18.89	6
ATOM	2014	CB	LEU	A	253	30.352	31.944	65.695	1.00	20.05	6
ATOM	2015	CG	LEU	A	253	29.198	32.942	65.842	1.00	21.61	6
ATOM	2016	CD1	LEU	A	253	27.849	32.220	65.860	1.00	22.23	6
ATOM	2017	CD2	LEU	A	253	29.395	33.716	67.145	1.00	22.90	6
ATOM	2018	C	LEU	A	253	30.539	31.901	63.198	1.00	20.05	6
ATOM	2019	O	LEU	A	253	31.466	32.691	62.987	1.00	18.17	8
ATOM	2020	N	GLN	A	254	29.544	31.720	62.340	1.00	19.40	7
ATOM	2021	CA	GLN	A	254	29.488	32.490	61.115	1.00	18.17	6
ATOM	2022	CB	GLN	A	254	29.017	31.592	59.969	1.00	9.67	6
ATOM	2023	CG	GLN	A	254	27.584	31.713	59.601	1.00	18.43	6
ATOM	2024	CD	GLN	A	254	27.368	32.766	58.549	1.00	19.97	6
ATOM	2025	OE1	GLN	A	254	27.917	32.677	57.450	1.00	22.54	8
ATOM	2026	NE2	GLN	A	254	26.564	33.769	58.869	1.00	22.89	7
ATOM	2027	C	GLN	A	254	28.520	33.634	61.444	1.00	19.75	6
ATOM	2028	O	GLN	A	254	27.470	33.415	62.060	1.00	18.77	8
ATOM	2029	N	LEU	A	255	28.905	34.854	61.067	1.00	23.02	7
ATOM	2030	CA	LEU	A	255	28.132	36.052	61.369	1.00	23.77	6
ATOM	2031	CB	LEU	A	255	28.963	36.993	62.242	1.00	26.84	5
ATOM	2032	CG	LEU	A	255	29.226	36.556	63.684	1.00	29.34	6
ATOM	2033	CD1	LEU	A	255	30.196	37.520	64.331	1.00	30.65	6
ATOM	2034	CD2	LEU	A	255	27.902	36.506	64.456	1.00	28.42	6
ATOM	2035	C	LEU	A	255	27.605	36.842	60.197	1.00	24.84	6
ATOM	2036	O	LEU	A	255	27.774	38.066	60.149	1.00	24.94	8
ATOM	2037	N	GLY	A	256	26.969	36.158	59.254	1.00	25.07	7
ATOM	2038	CA	GLY	A	256	26.408	36.858	58.117	1.00	26.11	6
ATOM	2039	C	GLY	A	256	25.506	37.956	58.644	1.00	27.11	6
ATOM	2040	O	GLY	A	256	24.742	37.734	59.584	1.00	25.67	8
ATOM	2041	N	THR	A	257	25.599	39.150	58.072	1.00	27.85	7
ATOM	2042	CA	THR	A	257	24.757	40.244	58.536	1.00	29.28	6
ATOM	2043	CB	THR	A	257	25.517	41.597	58.545	1.00	27.98	6
ATOM	2044	OG1	THR	A	257	26.002	41.895	57.232	1.00	31.91	8
ATOM	2045	CG2	THR	A	257	26.686	41.541	59.510	1.00	26.45	6
ATOM	2046	C	THR	A	257	23.477	40.392	57.722	1.00	28.39	6

Figure 17-32

ATOM	2047	O	THR	A	257	22.747	41.370	57.879	1.00	29.49	8
ATOM	2048	N	ASP	A	258	23.192	39.414	56.867	1.00	29.13	7
ATOM	2049	CA	ASP	A	258	21.977	39.471	56.065	1.00	30.49	6
ATOM	2050	CB	ASP	A	258	22.004	38.432	54.933	1.00	28.22	6
ATOM	2051	CG	ASP	A	258	22.337	37.033	55.416	1.00	29.39	6
ATOM	2052	OD1	ASP	A	258	21.893	36.653	56.520	1.00	30.16	8
ATOM	2053	OD2	ASP	A	258	23.019	36.292	54.667	1.00	29.97	8
ATOM	2054	C	ASP	A	258	20.646	39.355	56.826	1.00	30.50	6
ATOM	2055	O	ASP	A	258	19.601	39.622	56.248	1.00	32.87	8
ATOM	2056	N	PRO	A	259	20.650	38.912	58.101	1.00	30.76	7
ATOM	2057	CD	PRO	A	259	21.711	38.338	58.952	1.00	33.56	6
ATOM	2058	CA	PRO	A	259	19.366	38.821	58.806	1.00	31.73	6
ATOM	2059	CB	PRO	A	259	19.705	37.912	59.987	1.00	31.87	6
ATOM	2060	CG	PRO	A	259	21.067	38.373	60.333	1.00	31.73	6
ATOM	2061	C	PRO	A	259	18.817	40.184	59.260	1.00	30.86	6
ATOM	2062	O	PRO	A	259	17.736	40.270	59.845	1.00	29.78	8
ATOM	2063	N	LEU	A	260	19.565	41.245	58.980	1.00	29.58	7
ATOM	2064	CA	LEU	A	260	19.161	42.592	59.375	1.00	29.15	6
ATOM	2065	CB	LEU	A	260	20.367	43.542	59.275	1.00	27.14	6
ATOM	2066	CG	LEU	A	260	21.543	43.286	60.234	1.00	22.17	6
ATOM	2067	CD1	LEU	A	260	22.794	43.919	59.684	1.00	15.79	6
ATOM	2068	CD2	LEU	A	260	21.211	43.793	61.633	1.00	16.25	6
ATOM	2069	C	LEU	A	260	17.992	43.165	58.576	1.00	28.09	6
ATOM	2070	O	LEU	A	260	17.787	42.834	57.410	1.00	29.61	8
ATOM	2071	N	LEU	A	261	17.237	44.044	59.223	1.00	29.29	7
ATOM	2072	CA	LEU	A	261	16.097	44.693	58.596	1.00	29.71	6
ATOM	2073	CB	LEU	A	261	15.540	45.788	59.513	1.00	29.62	6
ATOM	2074	CG	LEU	A	261	14.406	46.664	58.950	1.00	28.14	6
ATOM	2075	CD1	LEU	A	261	13.144	45.819	58.803	1.00	24.82	6
ATOM	2076	CD2	LEU	A	261	14.139	47.859	59.882	1.00	25.45	6
ATOM	2077	C	LEU	A	261	16.461	45.322	57.259	1.00	29.50	6
ATOM	2078	O	LEU	A	261	15.717	45.198	56.295	1.00	31.67	8
ATOM	2079	N	GLU	A	262	17.603	45.998	57.201	1.00	31.54	7
ATOM	2080	CA	GLU	A	262	18.015	46.664	55.973	1.00	31.93	6
ATOM	2081	CB	GLU	A	262	19.049	47.758	56.279	1.00	29.34	6
ATOM	2082	CG	GLU	A	262	18.496	48.931	57.086	1.00	28.52	6
ATOM	2083	CD	GLU	A	262	18.449	48.687	58.589	1.00	29.76	6
ATOM	2084	OE1	GLU	A	262	18.175	47.548	59.029	1.00	30.12	8
ATOM	2085	OE2	GLU	A	262	18.661	49.661	59.338	1.00	27.69	8
ATOM	2086	C	GLU	A	262	18.526	45.754	54.857	1.00	34.29	6
ATOM	2087	O	GLU	A	262	18.690	46.199	53.722	1.00	35.20	8
ATOM	2088	N	ASP	A	263	18.778	44.486	55.158	1.00	36.55	7
ATOM	2089	CA	ASP	A	263	19.245	43.582	54.117	1.00	39.50	6
ATOM	2090	CB	ASP	A	263	20.354	42.672	54.641	1.00	38.42	6
ATOM	2091	CG	ASP	A	263	20.982	41.847	53.538	1.00	39.33	6
ATOM	2092	OD1	ASP	A	263	22.064	41.263	53.762	1.00	38.86	8
ATOM	2093	OD2	ASP	A	263	20.384	41.779	52.443	1.00	39.50	8
ATOM	2094	C	ASP	A	263	18.046	42.775	53.634	1.00	42.83	6
ATOM	2095	O	ASP	A	263	17.474	41.966	54.381	1.00	44.22	8
ATOM	2096	N	TYR	A	264	17.673	43.002	52.377	1.00	44.14	7
ATOM	2097	CA	TYR	A	264	16.508	42.357	51.796	1.00	46.67	6
ATOM	2098	CB	TYR	A	264	16.031	43.149	50.568	1.00	54.61	6
ATOM	2099	CG	TYR	A	264	16.824	42.939	49.294	1.00	63.02	6
ATOM	2100	CD1	TYR	A	264	16.510	41.897	48.412	1.00	65.73	6
ATOM	2101	CE1	TYR	A	264	17.230	41.709	47.226	1.00	68.35	6
ATOM	2102	CD2	TYR	A	264	17.882	43.786	48.962	1.00	66.23	6
ATOM	2103	CE2	TYR	A	264	18.611	43.606	47.780	1.00	68.63	6
ATOM	2104	CE	TYR	A	264	18.279	42.570	46.918	1.00	69.08	6
ATOM	2105	OH	TYR	A	264	18.989	42.411	45.746	1.00	69.01	8
ATOM	2106	C	TYR	A	264	16.665	40.888	51.451	1.00	43.89	6
ATOM	2107	O	TYR	A	264	15.663	40.185	51.293	1.00	44.80	8
ATOM	2108	N	LEU	A	265	17.897	40.400	51.333	1.00	40.37	7
ATOM	2109	CA	LEU	A	265	18.051	38.984	51.016	1.00	38.06	6
ATOM	2110	CB	LEU	A	265	19.474	38.646	50.538	1.00	33.48	6
ATOM	2111	CG	LEU	A	265	19.905	39.211	49.172	1.00	32.43	6
ATOM	2112	CD1	LEU	A	265	21.176	38.535	48.703	1.00	26.97	6

ATOM	2113	CD2	LEU A 265	18.828	38.954	48.141	1.00	34.41	6
ATOM	2114	C	LEU A 265	17.665	38.131	52.219	1.00	37.41	6
ATOM	2115	O	LEU A 265	18.125	37.000	52.370	1.00	37.96	8
ATOM	2116	N	SER A 266	16.804	38.694	53.066	1.00	36.21	7
ATOM	2117	CA	SER A 266	16.294	38.013	54.253	1.00	36.46	6
ATOM	2118	CB	SER A 266	17.263	38.136	55.427	1.00	37.22	6
ATOM	2119	OG	SER A 266	17.190	39.440	55.991	1.00	37.41	8
ATOM	2120	C	SER A 266	14.997	38.705	54.653	1.00	35.55	6
ATOM	2121	O	SER A 266	14.889	39.927	54.568	1.00	37.09	8
ATOM	2122	N	LYS A 267	14.018	37.928	55.093	1.00	34.33	7
ATOM	2123	CA	LYS A 267	12.750	38.493	55.532	1.00	36.13	6
ATOM	2124	CB	LYS A 267	11.596	37.548	55.183	1.00	36.11	6
ATOM	2125	CG	LYS A 267	11.503	37.222	53.705	1.00	36.79	6
ATOM	2126	CD	LYS A 267	11.453	38.487	52.869	1.00	38.55	6
ATOM	2127	CE	LYS A 267	11.369	38.170	51.389	1.00	41.60	6
ATOM	2128	NZ	LYS A 267	11.503	39.413	50.569	1.00	42.07	7
ATOM	2129	C	LYS A 267	12.791	38.738	57.043	1.00	34.90	6
ATOM	2130	O	LYS A 267	11.758	38.867	57.694	1.00	37.18	8
ATOM	2131	N	PHE A 268	13.998	38.775	57.595	1.00	32.82	7
ATOM	2132	CA	PHE A 268	14.192	39.021	59.016	1.00	31.50	6
ATOM	2133	CB	PHE A 268	15.477	38.337	59.495	1.00	34.05	6
ATOM	2134	CG	PHE A 268	15.379	36.839	59.604	1.00	34.54	6
ATOM	2135	CD1	PHE A 268	16.506	36.087	59.940	1.00	35.04	6
ATOM	2136	CD2	PHE A 268	14.161	36.178	59.429	1.00	34.57	6
ATOM	2137	CE1	PHE A 268	16.423	34.691	60.108	1.00	35.44	6
ATOM	2138	CE2	PHE A 268	14.066	34.784	59.594	1.00	36.00	6
ATOM	2139	CZ	PHE A 268	15.201	34.040	59.936	1.00	34.68	6
ATOM	2140	C	PHE A 268	14.319	40.530	59.190	1.00	30.94	6
ATOM	2141	O	PHE A 268	14.983	41.192	58.394	1.00	30.27	8
ATOM	2142	N	ASN A 269	13.693	41.081	60.222	1.00	32.53	7
ATOM	2143	CA	ASN A 269	13.760	42.527	60.448	1.00	35.83	6
ATOM	2144	CB	ASN A 269	12.344	43.115	60.570	1.00	37.23	6
ATOM	2145	CG	ASN A 269	11.478	42.809	59.360	1.00	40.75	6
ATOM	2146	OD1	ASN A 269	11.830	43.148	58.227	1.00	43.88	8
ATOM	2147	ND2	ASN A 269	10.335	42.165	59.594	1.00	39.61	7
ATOM	2148	C	ASN A 269	14.553	42.854	61.710	1.00	35.45	6
ATOM	2149	O	ASN A 269	14.095	43.621	62.560	1.00	41.47	8
ATOM	2150	N	LEU A 270	15.747	42.285	61.827	1.00	33.27	7
ATOM	2151	CA	LEU A 270	16.571	42.510	63.004	1.00	30.68	6
ATOM	2152	CB	LEU A 270	17.638	41.431	63.114	1.00	27.41	6
ATOM	2153	CG	LEU A 270	17.140	40.002	62.988	1.00	23.76	6
ATOM	2154	CD1	LEU A 270	18.222	39.106	63.543	1.00	27.14	6
ATOM	2155	CD2	LEU A 270	15.855	39.801	63.772	1.00	28.00	6
ATOM	2156	C	LEU A 270	17.258	43.856	63.033	1.00	32.30	6
ATOM	2157	O	LEU A 270	17.347	44.554	62.017	1.00	36.27	8
ATOM	2158	N	SER A 271	17.749	44.207	64.216	1.00	30.33	7
ATOM	2159	CA	SER A 271	18.465	45.457	64.424	1.00	30.79	6
ATOM	2160	CB	SER A 271	17.816	46.249	65.562	1.00	29.53	6
ATOM	2161	OG	SER A 271	17.712	45.471	66.739	1.00	30.43	8
ATOM	2162	C	SER A 271	19.911	45.109	64.768	1.00	33.09	6
ATOM	2163	O	SER A 271	20.194	43.972	65.172	1.00	29.64	8
ATOM	2164	N	ASN A 272	20.821	46.069	64.586	1.00	32.36	7
ATOM	2165	CA	ASN A 272	22.234	45.846	64.896	1.00	31.65	6
ATOM	2166	CB	ASN A 272	23.036	47.141	64.771	1.00	33.76	6
ATOM	2167	CG	ASN A 272	23.101	47.658	63.361	1.00	37.76	6
ATOM	2168	OD1	ASN A 272	23.719	48.686	63.100	1.00	36.12	8
ATOM	2169	ND2	ASN A 272	22.460	46.952	62.437	1.00	44.79	7
ATOM	2170	C	ASN A 272	22.369	45.333	66.321	1.00	32.61	6
ATOM	2171	O	ASN A 272	22.970	44.283	66.565	1.00	27.95	8
ATOM	2172	N	VAL A 273	21.803	46.091	67.257	1.00	33.22	7
ATOM	2173	CA	VAL A 273	21.839	45.741	68.668	1.00	35.52	6
ATOM	2174	CB	VAL A 273	20.928	46.660	69.481	1.00	37.80	6
ATOM	2175	CG1	VAL A 273	20.987	46.276	70.964	1.00	39.00	6
ATOM	2176	CG2	VAL A 273	21.356	48.112	69.275	1.00	38.88	6
ATOM	2177	C	VAL A 273	21.416	44.300	68.908	1.00	34.26	6
ATOM	2178	O	VAL A 273	22.060	43.580	69.679	1.00	35.96	8

ATOM	2179	N	ALA	A	274	20.328	43.889	68.262	1.00	32.36	7
ATOM	2180	CA	ALA	A	274	19.834	42.521	68.385	1.00	31.09	6
ATOM	2181	CB	ALA	A	274	18.574	42.356	67.578	1.00	28.88	6
ATOM	2182	C	ALA	A	274	20.923	41.588	67.861	1.00	31.74	6
ATOM	2183	O	ALA	A	274	21.323	40.634	68.533	1.00	31.54	8
ATOM	2184	N	PHE	A	275	21.401	41.879	66.655	1.00	30.05	7
ATOM	2185	CA	PHE	A	275	22.467	41.102	66.036	1.00	31.30	6
ATOM	2186	CB	PHE	A	275	22.932	41.810	64.751	1.00	31.54	6
ATOM	2187	CG	PHE	A	275	23.938	41.029	63.941	1.00	31.76	6
ATOM	2188	CD1	PHE	A	275	23.597	39.809	63.365	1.00	32.40	6
ATOM	2189	CD2	PHE	A	275	25.219	41.529	63.729	1.00	34.04	6
ATOM	2190	CE1	PHE	A	275	24.513	39.100	62.586	1.00	32.27	6
ATOM	2191	CE2	PHE	A	275	26.149	40.828	62.950	1.00	33.90	6
ATOM	2192	CZ	PHE	A	275	25.793	39.613	62.378	1.00	34.50	6
ATOM	2193	C	PHE	A	275	23.632	40.999	67.040	1.00	29.98	6
ATOM	2194	O	PHE	A	275	24.252	39.950	67.200	1.00	29.41	8
ATOM	2195	N	LEU	A	276	23.908	42.099	67.726	1.00	31.22	7
ATOM	2196	CA	LEU	A	276	24.988	42.144	68.698	1.00	32.29	6
ATOM	2197	CB	LEU	A	276	25.221	43.594	69.141	1.00	33.44	6
ATOM	2198	CG	LEU	A	276	26.415	43.908	70.050	1.00	36.01	6
ATOM	2199	CD1	LEU	A	276	26.683	45.391	70.025	1.00	35.02	6
ATOM	2200	CD2	LEU	A	276	26.147	43.433	71.467	1.00	39.09	6
ATOM	2201	C	LEU	A	276	24.682	41.244	69.894	1.00	32.79	6
ATOM	2202	O	LEU	A	276	25.560	40.530	70.371	1.00	30.74	8
ATOM	2203	N	LYS	A	277	23.445	41.273	70.384	1.00	33.95	7
ATOM	2204	CA	LYS	A	277	23.086	40.413	71.505	1.00	36.56	6
ATOM	2205	CB	LYS	A	277	21.623	40.588	71.902	1.00	35.76	6
ATOM	2206	CG	LYS	A	277	21.343	41.842	72.687	1.00	42.31	6
ATOM	2207	CD	LYS	A	277	20.743	41.508	74.049	1.00	45.72	6
ATOM	2208	CE	LYS	A	277	21.665	40.601	74.865	1.00	47.87	6
ATOM	2209	NZ	LYS	A	277	21.140	40.378	76.244	1.00	44.36	7
ATOM	2210	C	LYS	A	277	23.302	38.974	71.092	1.00	37.98	6
ATOM	2211	O	LYS	A	277	23.875	38.179	71.845	1.00	37.54	8
ATOM	2212	N	ALA	A	278	22.832	38.654	69.886	1.00	37.17	7
ATOM	2213	CA	ALA	A	278	22.952	37.311	69.323	1.00	34.51	6
ATOM	2214	CB	ALA	A	278	22.638	37.341	67.820	1.00	35.38	6
ATOM	2215	C	ALA	A	278	24.368	36.831	69.550	1.00	30.63	6
ATOM	2216	O	ALA	A	278	24.605	35.790	70.167	1.00	27.62	8
ATOM	2217	N	PHE	A	279	25.303	37.624	69.049	1.00	29.24	7
ATOM	2218	CA	PHE	A	279	26.722	37.347	69.167	1.00	31.48	6
ATOM	2219	CB	PHE	A	279	27.490	38.558	68.645	1.00	33.25	6
ATOM	2220	CG	PHE	A	279	28.974	38.396	68.663	1.00	39.28	6
ATOM	2221	CD1	PHE	A	279	29.578	37.337	68.000	1.00	41.15	6
ATOM	2222	CD2	PHE	A	279	29.776	39.328	69.315	1.00	40.66	6
ATOM	2223	CE1	PHE	A	279	30.960	37.209	67.987	1.00	44.22	6
ATOM	2224	CE2	PHE	A	279	31.153	39.213	69.378	1.00	41.38	6
ATOM	2225	CZ	PHE	A	279	31.750	38.152	68.614	1.00	44.52	6
ATOM	2226	C	PHE	A	279	27.116	37.043	70.611	1.00	31.81	6
ATOM	2227	O	PHE	A	279	27.627	35.953	70.935	1.00	27.51	8
ATOM	2228	N	ASN	A	280	26.860	38.005	71.503	1.00	29.32	7
ATOM	2229	CA	ASN	A	280	27.192	37.851	72.907	1.00	29.26	6
ATOM	2230	CB	ASN	A	280	26.927	39.153	73.660	1.00	30.39	6
ATOM	2231	CG	ASN	A	280	27.907	40.245	73.278	1.00	30.68	6
ATOM	2232	OD1	ASN	A	280	29.117	40.030	73.303	1.00	33.34	8
ATOM	2233	ND2	ASN	A	280	27.395	41.419	72.931	1.00	27.00	7
ATOM	2234	C	ASN	A	280	26.524	36.680	73.616	1.00	30.01	6
ATOM	2235	O	ASN	A	280	27.167	36.004	74.419	1.00	29.58	8
ATOM	2236	N	ILE	A	281	25.252	36.423	73.335	1.00	30.46	7
ATOM	2237	CA	ILE	A	281	24.594	35.291	73.983	1.00	33.71	6
ATOM	2238	CB	ILE	A	281	23.107	35.161	73.569	1.00	36.14	6
ATOM	2239	CG2	ILE	A	281	22.541	33.820	74.032	1.00	36.18	6
ATOM	2240	CG1	ILE	A	281	22.298	36.307	74.177	1.00	33.52	6
ATOM	2241	CD1	ILE	A	281	20.835	36.243	73.834	1.00	37.16	6
ATOM	2242	C	ILE	A	281	25.330	34.006	73.631	1.00	34.06	6
ATOM	2243	O	ILE	A	281	25.385	33.071	74.437	1.00	31.94	8
ATOM	2244	N	VAL	A	282	25.896	33.960	72.427	1.00	35.31	7

ATOM	2245	CA	VAL	A	282	26.654	32.785	72.005	1.00	36.45	6
ATOM	2246	CB	VAL	A	282	27.084	32.871	70.524	1.00	35.62	6
ATOM	2247	CG1	VAL	A	282	27.829	31.604	70.126	1.00	31.20	6
ATOM	2248	CG2	VAL	A	282	25.880	33.080	69.646	1.00	34.51	6
ATOM	2249	C	VAL	A	282	27.919	32.723	72.857	1.00	37.80	6
ATOM	2250	O	VAL	A	282	28.182	31.722	73.532	1.00	36.12	8
ATOM	2251	N	ARG	A	283	28.693	33.808	72.821	1.00	38.45	7
ATOM	2252	CA	ARG	A	283	29.929	33.884	73.587	1.00	40.06	6
ATOM	2253	CB	ARG	A	283	30.551	35.272	73.449	1.00	39.38	6
ATOM	2254	CG	ARG	A	283	30.974	35.625	72.027	1.00	41.90	6
ATOM	2255	CD	ARG	A	283	31.492	37.048	71.968	1.00	41.36	6
ATOM	2256	NE	ARG	A	283	32.647	37.206	72.840	1.00	43.35	7
ATOM	2257	CZ	ARG	A	283	33.162	38.373	73.215	1.00	42.55	6
ATOM	2258	NH1	ARG	A	283	32.628	39.516	72.797	1.00	39.95	7
ATOM	2259	NH2	ARG	A	283	34.220	38.392	74.014	1.00	41.72	7
ATOM	2260	C	ARG	A	283	29.614	33.587	75.044	1.00	40.01	6
ATOM	2261	O	ARG	A	283	30.350	32.862	75.716	1.00	39.01	8
ATOM	2262	N	GLU	A	284	28.506	34.141	75.520	1.00	40.30	7
ATOM	2263	CA	GLU	A	284	28.084	33.923	76.894	1.00	43.19	6
ATOM	2264	CB	GLU	A	284	26.753	34.647	77.165	1.00	47.53	6
ATOM	2265	CG	GLU	A	284	26.875	36.176	77.090	1.00	56.10	6
ATOM	2266	CD	GLU	A	284	25.542	36.923	77.179	1.00	60.77	6
ATOM	2267	OE1	GLU	A	284	24.659	36.682	76.329	1.00	61.41	8
ATOM	2268	OE2	GLU	A	284	25.383	37.763	78.096	1.00	62.21	8
ATOM	2269	C	GLU	A	284	27.953	32.429	77.179	1.00	40.72	6
ATOM	2270	O	GLU	A	284	28.565	31.922	78.120	1.00	45.29	8
ATOM	2271	N	VAL	A	285	27.186	31.721	76.354	1.00	34.82	7
ATOM	2272	CA	VAL	A	285	26.975	30.288	76.551	1.00	30.84	6
ATOM	2273	CB	VAL	A	285	25.842	29.752	75.647	1.00	27.74	6
ATOM	2274	CG1	VAL	A	285	25.698	28.253	75.831	1.00	22.95	6
ATOM	2275	CG2	VAL	A	285	24.545	30.433	75.982	1.00	26.26	6
ATOM	2276	C	VAL	A	285	28.181	29.366	76.341	1.00	31.93	6
ATOM	2277	O	VAL	A	285	28.492	28.556	77.214	1.00	33.46	8
ATOM	2278	N	PHE	A	286	28.845	29.466	75.191	1.00	29.43	7
ATOM	2279	CA	PHE	A	286	29.973	28.586	74.907	1.00	24.26	6
ATOM	2280	CB	PHE	A	286	29.830	27.957	73.519	1.00	22.57	6
ATOM	2281	CG	PHE	A	286	28.607	27.095	73.345	1.00	23.46	6
ATOM	2282	CD1	PHE	A	286	27.409	27.639	72.885	1.00	23.90	6
ATOM	2283	CD2	PHE	A	286	28.664	25.718	73.608	1.00	21.95	6
ATOM	2284	CE1	PHE	A	286	26.281	26.814	72.681	1.00	24.90	6
ATOM	2285	CE2	PHE	A	286	27.547	24.892	73.411	1.00	18.06	6
ATOM	2286	CZ	PHE	A	286	26.357	25.437	72.945	1.00	20.23	6
ATOM	2287	C	PHE	A	286	31.368	29.200	74.991	1.00	25.14	6
ATOM	2288	O	PHE	A	286	32.338	28.566	74.560	1.00	23.16	8
ATOM	2289	N	GLY	A	287	31.480	30.416	75.525	1.00	25.51	7
ATOM	2290	CA	GLY	A	287	32.783	31.065	75.614	1.00	26.86	6
ATOM	2291	C	GLY	A	287	33.353	31.511	74.270	1.00	26.28	6
ATOM	2292	O	GLY	A	287	32.644	31.549	73.271	1.00	26.29	8
ATOM	2293	N	GLU	A	288	34.637	31.849	74.238	1.00	27.17	7
ATOM	2294	CA	GLU	A	288	35.274	32.291	72.996	1.00	33.20	6
ATOM	2295	CB	GLU	A	288	36.680	32.828	73.269	1.00	35.09	6
ATOM	2296	CG	GLU	A	288	36.726	34.104	74.083	1.00	41.67	6
ATOM	2297	CD	GLU	A	288	35.970	35.231	73.421	1.00	43.13	6
ATOM	2298	OE1	GLU	A	288	36.221	35.493	72.228	1.00	45.39	8
ATOM	2299	OE2	GLU	A	288	35.130	35.858	74.097	1.00	47.64	8
ATOM	2300	C	GLU	A	288	35.386	31.204	71.930	1.00	32.87	6
ATOM	2301	O	GLU	A	288	35.596	30.029	72.247	1.00	31.59	8
ATOM	2302	N	GLY	A	289	35.268	31.619	70.668	1.00	31.93	7
ATOM	2303	CA	GLY	A	289	35.373	30.698	69.545	1.00	29.58	6
ATOM	2304	C	GLY	A	289	35.948	31.372	68.307	1.00	27.42	6
ATOM	2305	O	GLY	A	289	36.556	32.437	68.398	1.00	26.27	6
ATOM	2306	N	VAL	A	290	35.764	30.758	67.143	1.00	27.64	7
ATOM	2307	CA	VAL	A	290	36.277	31.349	65.907	1.00	27.17	6
ATOM	2308	CB	VAL	A	290	37.014	30.301	65.037	1.00	25.25	6
ATOM	2309	CG1	VAL	A	290	37.616	30.976	63.813	1.00	22.41	6
ATOM	2310	CG2	VAL	A	290	38.100	29.632	65.852	1.00	17.33	6

Figure 17-36

ATOM	2311	C	VAL	A	290	35.137	31.975	65.105	1.00	25.97	6
ATOM	2312	O	VAL	A	290	34.218	31.279	64.672	1.00	22.32	8
ATOM	2313	N	TYR	A	291	35.217	33.293	64.914	1.00	27.33	7
ATOM	2314	CA	TYR	A	291	34.188	34.052	64.203	1.00	26.69	6
ATOM	2315	CB	TYR	A	291	33.925	35.356	64.939	1.00	25.51	6
ATOM	2316	CG	TYR	A	291	33.935	35.178	66.435	1.00	28.73	6
ATOM	2317	CD1	TYR	A	291	35.025	35.596	67.191	1.00	29.72	6
ATOM	2318	CE1	TYR	A	291	35.059	35.414	68.563	1.00	29.53	6
ATOM	2319	CD2	TYR	A	291	32.874	34.565	67.094	1.00	27.39	6
ATOM	2320	CE2	TYR	A	291	32.898	34.377	68.466	1.00	31.03	6
ATOM	2321	CZ	TYR	A	291	33.997	34.808	69.194	1.00	31.85	6
ATOM	2322	OH	TYR	A	291	34.030	34.647	70.562	1.00	38.03	8
ATOM	2323	C	TYR	A	291	34.527	34.345	62.745	1.00	27.99	6
ATOM	2324	O	TYR	A	291	35.608	34.843	62.415	1.00	24.83	8
ATOM	2325	N	LEU	A	292	33.567	34.042	61.880	1.00	30.17	7
ATOM	2326	CA	LEU	A	292	33.726	34.220	60.441	1.00	28.26	6
ATOM	2327	CB	LEU	A	292	33.561	32.861	59.741	1.00	27.70	6
ATOM	2328	CG	LEU	A	292	34.191	31.643	60.435	1.00	24.64	6
ATOM	2329	CD1	LEU	A	292	33.867	30.380	59.661	1.00	24.66	6
ATOM	2330	CD2	LEU	A	292	35.686	31.825	60.553	1.00	23.19	6
ATOM	2331	C	LEU	A	292	32.649	35.175	59.944	1.00	25.59	6
ATOM	2332	O	LEU	A	292	31.640	35.394	60.611	1.00	18.11	8
ATOM	2333	N	GLY	A	293	32.869	35.749	58.770	1.00	28.55	7
ATOM	2334	CA	GLY	A	293	31.878	36.653	58.223	1.00	31.26	6
ATOM	2335	C	GLY	A	293	30.722	35.815	57.714	1.00	34.84	6
ATOM	2336	O	GLY	A	293	30.463	34.724	58.234	1.00	34.11	8
ATOM	2337	N	GLY	A	294	30.036	36.312	56.689	1.00	35.34	7
ATOM	2338	CA	GLY	A	294	28.918	35.581	56.124	1.00	34.84	6
ATOM	2339	C	GLY	A	294	28.142	36.445	55.155	1.00	34.79	6
ATOM	2340	O	GLY	A	294	28.644	37.473	54.699	1.00	37.05	8
ATOM	2341	N	GLY	A	295	26.917	36.035	54.842	1.00	31.87	7
ATOM	2342	CA	GLY	A	295	26.102	36.806	53.925	1.00	27.78	6
ATOM	2343	C	GLY	A	295	25.969	38.245	54.378	1.00	27.09	6
ATOM	2344	O	GLY	A	295	26.192	38.558	55.546	1.00	27.03	8
ATOM	2345	N	GLY	A	296	25.596	39.119	53.450	1.00	24.67	7
ATOM	2346	CA	GLY	A	296	25.440	40.527	53.757	1.00	25.28	6
ATOM	2347	C	GLY	A	296	25.562	41.262	52.446	1.00	27.64	6
ATOM	2348	O	GLY	A	296	26.591	41.163	51.771	1.00	26.65	8
ATOM	2349	N	TYR	A	297	24.526	42.009	52.078	1.00	30.21	7
ATOM	2350	CA	TYR	A	297	24.543	42.704	50.801	1.00	30.62	6
ATOM	2351	CB	TYR	A	297	23.560	42.011	49.859	1.00	29.50	6
ATOM	2352	CG	TYR	A	297	23.717	40.516	49.953	1.00	30.33	6
ATOM	2353	CD1	TYR	A	297	23.174	39.810	51.031	1.00	30.86	6
ATOM	2354	CE1	TYR	A	297	23.450	38.449	51.226	1.00	30.74	6
ATOM	2355	CD2	TYR	A	297	24.538	39.824	49.062	1.00	31.20	6
ATOM	2356	CE2	TYR	A	297	24.821	38.460	49.247	1.00	32.08	6
ATOM	2357	CZ	TYR	A	297	24.275	37.781	50.332	1.00	30.92	6
ATOM	2358	OH	TYR	A	297	24.539	36.440	50.509	1.00	29.60	8
ATOM	2359	C	TYR	A	297	24.267	44.195	50.875	1.00	32.07	6
ATOM	2360	O	TYR	A	297	24.134	44.849	49.840	1.00	33.83	8
ATOM	2361	N	HIS	A	298	24.180	44.725	52.094	1.00	31.41	7
ATOM	2362	CA	HIS	A	298	23.961	46.153	52.289	1.00	33.94	6
ATOM	2363	CB	HIS	A	298	22.761	46.430	53.194	1.00	34.75	6
ATOM	2364	CG	HIS	A	298	22.379	47.880	53.256	1.00	35.16	6
ATOM	2365	CD2	HIS	A	298	22.558	48.809	54.224	1.00	35.72	6
ATOM	2366	ND1	HIS	A	298	21.779	48.538	52.205	1.00	34.10	7
ATOM	2367	CE1	HIS	A	298	21.605	49.809	52.522	1.00	31.84	6
ATOM	2368	NE2	HIS	A	298	22.069	50.000	53.742	1.00	35.46	7
ATOM	2369	C	HIS	A	298	25.213	46.697	52.962	1.00	36.21	6
ATOM	2370	O	HIS	A	298	25.471	46.405	54.133	1.00	33.83	8
ATOM	2371	N	PRO	A	299	25.992	47.519	52.234	1.00	36.69	7
ATOM	2372	CD	PRO	A	299	25.680	47.997	50.881	1.00	35.57	6
ATOM	2373	CA	PRO	A	299	27.238	48.142	52.689	1.00	36.17	6
ATOM	2374	CB	PRO	A	299	27.586	49.073	51.525	1.00	37.75	6
ATOM	2375	CG	PRO	A	299	26.216	49.399	50.954	1.00	37.76	6
ATOM	2376	C	PRO	A	299	27.045	48.886	54.000	1.00	34.47	6

Figure 17-37

ATOM	2377	O	PRO	A	299	27.781	48.670	54.963	1.00	33.67	8
ATOM	2378	N	TYR	A	300	26.051	49.763	54.026	1.00	32.69	7
ATOM	2379	CA	TYR	A	300	25.745	50.521	55.227	1.00	32.97	6
ATOM	2380	CB	TYR	A	300	24.496	51.377	55.009	1.00	35.56	6
ATOM	2381	CG	TYR	A	300	24.648	52.524	54.028	1.00	35.96	6
ATOM	2382	CD1	TYR	A	300	25.370	52.367	52.842	1.00	39.37	6
ATOM	2383	CE1	TYR	A	300	25.461	53.405	51.907	1.00	39.92	6
ATOM	2384	CD2	TYR	A	300	24.016	53.752	54.259	1.00	35.92	6
ATOM	2385	CE2	TYR	A	300	24.098	54.793	53.334	1.00	36.78	6
ATOM	2386	CZ	TYR	A	300	24.823	54.612	52.161	1.00	38.09	6
ATOM	2387	OH	TYR	A	300	24.927	55.634	51.251	1.00	37.68	8
ATOM	2388	C	TYR	A	300	25.497	49.546	56.369	1.00	31.10	6
ATOM	2389	O	TYR	A	300	26.062	49.692	57.440	1.00	30.62	8
ATOM	2390	N	ALA	A	301	24.661	48.541	56.125	1.00	32.55	7
ATOM	2391	CA	ALA	A	301	24.323	47.541	57.145	1.00	31.64	6
ATOM	2392	CB	ALA	A	301	23.216	46.602	56.624	1.00	24.69	6
ATOM	2393	C	ALA	A	301	25.539	46.727	57.552	1.00	30.06	6
ATOM	2394	O	ALA	A	301	25.848	46.579	58.734	1.00	31.91	8
ATOM	2395	N	LEU	A	302	26.223	46.192	56.557	1.00	28.94	7
ATOM	2396	CA	LEU	A	302	27.404	45.383	56.795	1.00	30.55	6
ATOM	2397	CB	LEU	A	302	28.012	45.002	55.441	1.00	31.83	6
ATOM	2398	CG	LEU	A	302	29.315	44.223	55.323	1.00	30.01	6
ATOM	2399	CD1	LEU	A	302	29.491	43.781	53.888	1.00	32.09	6
ATOM	2400	CD2	LEU	A	302	30.475	45.077	55.762	1.00	32.23	6
ATOM	2401	C	LEU	A	302	28.418	46.136	57.663	1.00	29.79	6
ATOM	2402	O	LEU	A	302	28.796	45.676	58.746	1.00	27.68	8
ATOM	2403	N	ALA	A	303	28.842	47.299	57.179	1.00	27.92	7
ATOM	2404	CA	ALA	A	303	29.818	48.119	57.877	1.00	25.00	6
ATOM	2405	CB	ALA	A	303	30.026	49.424	57.137	1.00	23.62	6
ATOM	2406	C	ALA	A	303	29.397	48.397	59.305	1.00	25.06	6
ATOM	2407	O	ALA	A	303	30.088	48.015	60.248	1.00	26.90	8
ATOM	2408	N	ARG	A	304	28.258	49.054	59.472	1.00	24.06	7
ATOM	2409	CA	ARG	A	304	27.794	49.382	60.810	1.00	24.37	6
ATOM	2410	CB	ARG	A	304	26.420	50.052	60.758	1.00	23.99	6
ATOM	2411	CG	ARG	A	304	26.328	51.257	59.815	1.00	28.77	6
ATOM	2412	CD	ARG	A	304	25.106	52.089	60.156	1.00	29.96	6
ATOM	2413	NE	ARG	A	304	23.943	51.233	60.369	1.00	36.43	7
ATOM	2414	CZ	ARG	A	304	22.893	51.573	61.110	1.00	37.01	6
ATOM	2415	NH1	ARG	A	304	22.854	52.757	61.713	1.00	36.37	7
ATOM	2416	NH2	ARG	A	304	21.896	50.719	61.269	1.00	34.36	7
ATOM	2417	C	ARG	A	304	27.727	48.142	61.691	1.00	24.24	6
ATOM	2418	O	ARG	A	304	28.343	48.099	62.762	1.00	22.34	8
ATOM	2419	N	ALA	A	305	26.994	47.132	61.221	1.00	24.51	7
ATOM	2420	CA	ALA	A	305	26.801	45.883	61.959	1.00	22.70	6
ATOM	2421	CB	ALA	A	305	25.880	44.960	61.175	1.00	18.13	6
ATOM	2422	C	ALA	A	305	28.089	45.142	62.351	1.00	23.33	6
ATOM	2423	O	ALA	A	305	28.237	44.725	63.506	1.00	21.51	8
ATOM	2424	N	TRP	A	306	29.016	44.961	61.411	1.00	22.79	7
ATOM	2425	CA	TRP	A	306	30.244	44.270	61.764	1.00	24.33	6
ATOM	2426	CB	TRP	A	306	31.029	43.842	60.524	1.00	26.93	6
ATOM	2427	CG	TRP	A	306	30.604	42.503	59.952	1.00	27.96	6
ATOM	2428	CD2	TRP	A	306	30.861	42.013	58.629	1.00	26.38	6
ATOM	2429	CE2	TRP	A	306	30.366	40.688	58.570	1.00	24.96	6
ATOM	2430	CE3	TRP	A	306	31.462	42.563	57.490	1.00	23.00	6
ATOM	2431	CD1	TRP	A	306	29.983	41.484	60.620	1.00	28.53	6
ATOM	2432	NE1	TRP	A	306	29.837	40.392	59.797	1.00	25.62	7
ATOM	2433	CZ2	TRP	A	306	30.450	39.904	57.414	1.00	24.51	6
ATOM	2434	CZ3	TRP	A	306	31.548	41.784	56.343	1.00	25.37	6
ATOM	2435	CH2	TRP	A	306	31.042	40.465	56.315	1.00	24.20	6
ATOM	2436	C	TRP	A	306	31.129	45.108	62.676	1.00	26.51	6
ATOM	2437	O	TRP	A	306	31.908	44.570	63.464	1.00	25.07	8
ATOM	2438	N	THR	A	307	31.003	46.427	62.575	1.00	28.08	7
ATOM	2439	CA	THR	A	307	31.785	47.323	63.415	1.00	27.91	6
ATOM	2440	CB	THR	A	307	31.484	48.796	63.100	1.00	27.86	6
ATOM	2441	CG1	THR	A	307	31.994	49.119	61.799	1.00	30.17	8
ATOM	2442	CG2	THR	A	307	32.120	49.704	64.137	1.00	24.72	6

Figure 17-38

ATOM	2443	C	THR	A	307	31.441	47.041	64.863	1.00	29.35	6
ATOM	2444	O	THR	A	307	32.316	46.989	65.725	1.00	32.56	8
ATOM	2445	N	LEU	A	308	30.159	46.857	65.135	1.00	30.60	7
ATOM	2446	CA	LEU	A	308	29.740	46.555	66.490	1.00	33.69	6
ATOM	2447	CB	LEU	A	308	28.256	46.215	66.525	1.00	34.48	6
ATOM	2448	CG	LEU	A	308	27.338	47.337	66.058	1.00	34.79	6
ATOM	2449	CD1	LEU	A	308	25.903	46.887	66.153	1.00	31.98	6
ATOM	2450	CD2	LEU	A	308	27.569	48.542	66.924	1.00	36.96	6
ATOM	2451	C	LEU	A	308	30.531	45.353	66.965	1.00	34.57	6
ATOM	2452	O	LEU	A	308	31.230	45.417	67.975	1.00	33.75	8
ATOM	2453	N	ILE	A	309	30.423	44.262	66.208	1.00	35.78	7
ATOM	2454	CA	ILE	A	309	31.108	43.017	66.540	1.00	35.87	6
ATOM	2455	CB	ILE	A	309	30.939	41.949	65.431	1.00	34.95	6
ATOM	2456	CG2	ILE	A	309	31.733	40.695	65.799	1.00	31.21	6
ATOM	2457	CG1	ILE	A	309	29.445	41.631	65.212	1.00	34.25	6
ATOM	2458	CD1	ILE	A	309	28.726	41.014	66.407	1.00	25.04	6
ATOM	2459	C	ILE	A	309	32.589	43.238	66.772	1.00	35.81	6
ATOM	2460	O	ILE	A	309	33.183	42.617	67.657	1.00	38.19	8
ATOM	2461	N	TRP	A	310	33.197	44.111	65.977	1.00	36.10	7
ATOM	2462	CA	TRP	A	310	34.612	44.384	66.169	1.00	35.26	6
ATOM	2463	CB	TRP	A	310	35.150	45.311	65.075	1.00	32.61	6
ATOM	2464	CG	TRP	A	310	36.619	45.588	65.220	1.00	30.79	6
ATOM	2465	CD2	TRP	A	310	37.679	44.620	65.274	1.00	29.93	6
ATOM	2466	CE2	TRP	A	310	38.882	45.330	65.474	1.00	28.42	6
ATOM	2467	CE3	TRP	A	310	37.731	43.224	65.174	1.00	31.59	6
ATOM	2468	CD1	TRP	A	310	37.206	46.804	65.380	1.00	30.62	6
ATOM	2469	NE1	TRP	A	310	38.565	46.659	65.536	1.00	29.37	7
ATOM	2470	CZ2	TRP	A	310	40.126	44.691	65.578	1.00	27.91	6
ATOM	2471	CZ3	TRP	A	310	38.978	42.585	65.279	1.00	28.06	6
ATOM	2472	CH2	TRP	A	310	40.150	43.322	65.479	1.00	26.50	6
ATOM	2473	C	TRP	A	310	34.744	45.040	67.545	1.00	36.00	6
ATOM	2474	O	TRP	A	310	35.365	44.476	68.440	1.00	36.24	8
ATOM	2475	N	CYS	A	311	34.134	46.213	67.715	1.00	34.57	7
ATOM	2476	CA	CYS	A	311	34.183	46.937	68.985	1.00	32.82	6
ATOM	2477	CB	CYS	A	311	33.169	48.085	68.996	1.00	35.62	6
ATOM	2478	SG	CYS	A	311	33.439	49.401	67.796	1.00	32.36	16
ATOM	2479	C	CYS	A	311	33.912	46.061	70.206	1.00	32.01	6
ATOM	2480	O	CYS	A	311	34.452	46.313	71.280	1.00	29.82	8
ATOM	2481	N	GLU	A	312	33.062	45.049	70.053	1.00	32.57	7
ATOM	2482	CA	GLU	A	312	32.731	44.159	71.171	1.00	33.86	6
ATOM	2483	CB	GLU	A	312	31.557	43.252	70.807	1.00	34.19	6
ATCM	2484	CG	GLU	A	312	30.442	43.185	71.844	1.00	40.27	6
ATOM	2485	CD	GLU	A	312	30.923	42.821	73.239	1.00	43.80	6
ATOM	2486	OE1	GLU	A	312	31.685	41.831	73.383	1.00	44.81	8
ATOM	2487	OE2	GLU	A	312	30.516	43.522	74.195	1.00	41.54	8
ATOM	2488	C	GLU	A	312	33.953	43.298	71.456	1.00	33.77	6
ATOM	2489	O	GLU	A	312	34.253	42.957	72.603	1.00	32.07	8
ATOM	2490	N	LEU	A	313	34.647	42.945	70.382	1.00	33.45	7
ATOM	2491	CA	LEU	A	313	35.848	42.135	70.473	1.00	32.89	6
ATOM	2492	CB	LEU	A	313	36.172	41.513	69.115	1.00	32.14	6
ATOM	2493	CG	LEU	A	313	35.154	40.493	68.626	1.00	27.73	6
ATOM	2494	CD1	LEU	A	313	35.587	39.956	67.269	1.00	30.39	6
ATOM	2495	CD2	LEU	A	313	35.053	39.367	69.648	1.00	27.87	6
ATOM	2496	C	LEU	A	313	36.976	43.031	70.903	1.00	31.64	6
ATOM	2497	O	LEU	A	313	37.605	42.793	71.925	1.00	31.74	8
ATCM	2498	N	SER	A	314	37.206	44.064	70.099	1.00	33.49	7
ATCM	2499	CA	SER	A	314	38.232	45.067	70.328	1.00	35.59	6
ATCM	2500	CB	SER	A	314	38.107	46.154	69.256	1.00	36.47	6
ATCM	2501	OG	SER	A	314	39.141	47.120	69.353	1.00	44.55	8
ATCM	2502	C	SER	A	314	38.046	45.661	71.730	1.00	37.82	6
ATCM	2503	O	SER	A	314	39.015	46.043	72.395	1.00	37.32	8
ATCM	2504	N	GLY	A	315	36.794	45.725	72.175	1.00	38.05	7
ATCM	2505	CA	GLY	A	315	36.506	46.243	73.498	1.00	42.42	6
ATCM	2506	C	GLY	A	315	36.295	47.744	73.568	1.00	46.80	6
ATCM	2507	O	GLY	A	315	35.923	48.276	74.618	1.00	47.85	8
ATCM	2508	N	ARG	A	316	36.518	48.438	72.458	1.00	48.90	7

ATOM	2509	CA	ARG	A	316	36.346	49.885	72.448	1.00	52.27	6
ATOM	2510	CB	ARG	A	316	37.144	50.479	71.283	1.00	53.60	6
ATOM	2511	CG	ARG	A	316	36.730	50.007	69.900	1.00	52.11	6
ATOM	2512	CD	ARG	A	316	37.734	50.514	68.870	1.00	53.76	6
ATOM	2513	NE	ARG	A	316	39.028	49.854	69.019	1.00	53.67	7
ATOM	2514	CZ	ARG	A	316	40.135	50.221	68.383	1.00	55.34	6
ATOM	2515	NH1	ARG	A	316	40.110	51.253	67.552	1.00	55.44	7
ATOM	2516	NH2	ARG	A	316	41.266	49.546	68.569	1.00	55.80	7
ATOM	2517	C	ARG	A	316	34.882	50.343	72.391	1.00	52.06	6
ATOM	2518	O	ARG	A	316	34.075	49.781	71.652	1.00	54.96	8
ATOM	2519	N	GLU	A	317	34.547	51.361	73.182	1.00	51.87	7
ATOM	2520	CA	GLU	A	317	33.185	51.900	73.222	1.00	52.67	6
ATOM	2521	CB	GLU	A	317	33.111	53.139	74.123	1.00	54.70	6
ATOM	2522	CG	GLU	A	317	32.549	52.901	75.527	1.00	60.94	6
ATOM	2523	CD	GLU	A	317	33.353	51.912	76.361	1.00	64.62	6
ATOM	2524	OE1	GLU	A	317	33.025	51.741	77.556	1.00	64.59	8
ATOM	2525	OE2	GLU	A	317	34.305	51.302	75.832	1.00	68.64	8
ATOM	2526	C	GLU	A	317	32.642	52.256	71.843	1.00	51.27	6
ATOM	2527	O	GLU	A	317	33.270	52.983	71.077	1.00	49.34	8
ATOM	2528	N	VAL	A	318	31.457	51.733	71.548	1.00	51.30	7
ATOM	2529	CA	VAL	A	318	30.780	51.962	70.280	1.00	48.80	6
ATOM	2530	CB	VAL	A	318	29.522	51.071	70.169	1.00	47.11	6
ATOM	2531	CG1	VAL	A	318	28.875	51.237	68.808	1.00	45.53	6
ATOM	2532	CG2	VAL	A	318	29.895	49.631	70.424	1.00	47.05	6
ATOM	2533	C	VAL	A	318	30.349	53.411	70.178	1.00	47.64	6
ATOM	2534	O	VAL	A	318	29.511	53.867	70.953	1.00	47.61	8
ATOM	2535	N	PRO	A	319	30.925	54.165	69.234	1.00	48.14	7
ATOM	2536	CD	PRO	A	319	31.960	53.836	68.247	1.00	48.87	6
ATOM	2537	CA	PRO	A	319	30.538	55.569	69.093	1.00	52.54	6
ATOM	2538	CB	PRO	A	319	31.438	56.051	67.954	1.00	49.96	6
ATOM	2539	CG	PRO	A	319	31.612	54.802	67.141	1.00	50.17	6
ATOM	2540	C	PRO	A	319	29.052	55.679	68.764	1.00	55.84	6
ATOM	2541	O	PRO	A	319	28.531	54.913	67.953	1.00	56.06	8
ATOM	2542	N	GLU	A	320	28.369	56.624	69.402	1.00	59.20	7
ATOM	2543	CA	GLU	A	320	26.942	56.804	69.167	1.00	62.61	6
ATOM	2544	CB	GLU	A	320	26.302	57.588	70.313	1.00	65.59	6
ATOM	2545	CG	GLU	A	320	26.727	59.042	70.365	1.00	73.01	6
ATOM	2546	CD	GLU	A	320	26.007	59.823	71.451	1.00	76.93	6
ATOM	2547	OE1	GLU	A	320	24.755	59.832	71.446	1.00	77.37	8
ATOM	2548	OE2	GLU	A	320	26.697	60.431	72.303	1.00	79.46	8
ATOM	2549	C	GLU	A	320	26.698	57.551	67.863	1.00	61.40	6
ATOM	2550	O	GLU	A	320	25.663	58.197	67.699	1.00	62.33	8
ATOM	2551	N	LYS	A	321	27.650	57.463	66.939	1.00	59.47	7
ATOM	2552	CA	LYS	A	321	27.519	58.150	65.662	1.00	59.54	6
ATOM	2553	CB	LYS	A	321	27.340	59.648	65.897	1.00	61.36	6
ATOM	2554	CG	LYS	A	321	27.620	60.323	66.366	1.00	65.23	6
ATOM	2555	CD	LYS	A	321	27.169	59.691	67.643	1.00	66.59	6
ATOM	2556	CE	LYS	A	321	27.564	60.215	67.960	1.00	67.34	6
ATOM	2557	NZ	LYS	A	321	30.591	61.699	68.100	1.00	68.58	7
ATOM	2558	C	LYS	A	321	28.766	57.941	64.806	1.00	59.24	6
ATOM	2559	O	LYS	A	321	29.845	57.623	65.319	1.00	58.70	8
ATOM	2560	N	LEU	A	322	28.608	58.146	63.500	1.00	57.55	7
ATOM	2561	CA	LEU	A	322	29.702	58.002	62.543	1.00	54.72	6
ATOM	2562	CB	LEU	A	322	29.171	57.450	61.214	1.00	52.96	6
ATOM	2563	CG	LEU	A	322	28.141	56.316	61.295	1.00	52.97	6
ATOM	2564	CD1	LEU	A	322	27.708	55.932	59.899	1.00	49.01	6
ATOM	2565	CD2	LEU	A	322	28.716	55.115	62.035	1.00	54.73	6
ATOM	2566	C	LEU	A	322	30.250	59.406	62.313	1.00	53.47	6
ATOM	2567	O	LEU	A	322	29.512	60.383	62.464	1.00	53.39	8
ATOM	2568	N	ASN	A	323	31.530	59.521	61.965	1.00	51.43	7
ATOM	2569	CA	ASN	A	323	32.089	60.842	61.706	1.00	50.32	6
ATOM	2570	CB	ASN	A	323	33.591	60.905	62.035	1.00	52.31	6
ATOM	2571	CG	ASN	A	323	34.428	59.964	61.189	1.00	55.06	6
ATOM	2572	OD1	ASN	A	323	34.386	58.744	61.363	1.00	55.77	8
ATOM	2573	ND2	ASN	A	323	35.195	60.530	60.259	1.00	52.71	7
ATOM	2574	C	ASN	A	323	31.843	61.199	60.243	1.00	48.63	6

107/263

Figure 17-40

ATOM	2575	O	ASN A 323	31.135	60.479	59.538	1.00	47.52	8
ATOM	2576	N	ASN A 324	32.426	62.304	59.792	1.00	47.66	7
ATOM	2577	CA	ASN A 324	32.242	62.769	58.419	1.00	49.25	6
ATOM	2578	CB	ASN A 324	32.758	64.200	58.292	1.00	50.73	6
ATOM	2579	CG	ASN A 324	32.025	65.154	59.205	1.00	53.83	6
ATOM	2580	OD1	ASN A 324	30.812	65.314	59.096	1.00	56.90	8
ATOM	2581	ND2	ASN A 324	32.755	65.789	60.119	1.00	54.93	7
ATOM	2582	C	ASN A 324	32.906	61.891	57.367	1.00	49.34	6
ATOM	2583	O	ASN A 324	32.275	61.502	56.379	1.00	47.22	8
ATOM	2584	N	LYS A 325	34.182	61.590	57.586	1.00	48.27	7
ATOM	2585	CA	LYS A 325	34.957	60.759	56.676	1.00	46.57	6
ATOM	2586	CB	LYS A 325	36.314	60.453	57.305	1.00	49.94	6
ATOM	2587	CG	LYS A 325	37.299	59.737	56.399	1.00	54.75	6
ATOM	2588	CD	LYS A 325	38.562	59.329	57.173	1.00	58.22	6
ATOM	2589	CE	LYS A 325	39.236	60.521	57.844	1.00	58.35	6
ATOM	2590	NZ	LYS A 325	40.473	60.128	58.566	1.00	59.81	7
ATOM	2591	C	LYS A 325	34.202	59.458	56.410	1.00	44.85	6
ATOM	2592	O	LYS A 325	34.065	59.027	55.263	1.00	43.59	8
ATOM	2593	N	ALA A 326	33.712	58.843	57.483	1.00	42.27	7
ATOM	2594	CA	ALA A 326	32.964	57.597	57.387	1.00	40.91	6
ATOM	2595	CB	ALA A 326	32.663	57.067	58.773	1.00	36.86	6
ATOM	2596	C	ALA A 326	31.666	57.803	56.612	1.00	43.30	6
ATOM	2597	O	ALA A 326	31.342	57.028	55.705	1.00	42.83	8
ATOM	2598	N	LYS A 327	30.918	58.843	56.977	1.00	45.56	7
ATOM	2599	CA	LYS A 327	29.657	59.146	56.306	1.00	47.23	6
ATOM	2600	CB	LYS A 327	29.023	60.407	56.892	1.00	49.59	6
ATOM	2601	CG	LYS A 327	28.547	60.263	58.329	1.00	54.63	6
ATOM	2602	CD	LYS A 327	28.024	61.591	58.862	1.00	55.89	6
ATOM	2603	CE	LYS A 327	27.529	61.483	60.299	1.00	58.28	6
ATOM	2604	NZ	LYS A 327	26.304	60.644	60.426	1.00	59.91	7
ATOM	2605	C	LYS A 327	29.888	59.347	54.816	1.00	46.97	6
ATOM	2606	O	LYS A 327	29.090	58.913	53.990	1.00	48.10	8
ATOM	2607	N	GLU A 328	30.986	60.012	54.480	1.00	44.99	7
ATOM	2608	CA	GLU A 328	31.325	60.264	53.091	1.00	43.18	6
ATOM	2609	CB	GLU A 328	32.417	61.326	53.027	1.00	47.93	6
ATOM	2610	CG	GLU A 328	31.993	62.621	53.710	1.00	53.65	6
ATOM	2611	CD	GLU A 328	33.112	63.630	53.831	1.00	55.79	6
ATOM	2612	OE1	GLU A 328	33.642	64.060	52.783	1.00	58.73	8
ATOM	2613	OE2	GLU A 328	33.459	63.991	54.979	1.00	58.13	8
ATOM	2614	C	GLU A 328	31.789	58.971	52.437	1.00	41.56	6
ATOM	2615	O	GLU A 328	31.537	58.743	51.255	1.00	39.41	8
ATOM	2616	N	LEU A 329	32.465	58.123	53.211	1.00	40.64	7
ATOM	2617	CA	LEU A 329	32.940	56.844	52.695	1.00	36.45	6
ATOM	2618	CB	LEU A 329	33.623	56.032	53.801	1.00	34.70	6
ATOM	2619	CG	LEU A 329	34.100	54.610	53.433	1.00	35.69	6
ATOM	2620	CD1	LEU A 329	35.195	54.642	52.359	1.00	30.11	6
ATOM	2621	CD2	LEU A 329	34.619	53.926	54.683	1.00	34.63	6
ATOM	2622	C	LEU A 329	31.746	56.064	52.157	1.00	35.77	6
ATOM	2623	O	LEU A 329	31.692	55.746	50.975	1.00	34.94	8
ATOM	2624	N	LEU A 330	30.784	55.770	53.029	1.00	34.78	7
ATOM	2625	CA	LEU A 330	29.599	55.028	52.630	1.00	34.95	6
ATOM	2626	CB	LEU A 330	28.631	54.914	53.803	1.00	30.95	6
ATOM	2627	CG	LEU A 330	29.164	54.115	54.991	1.00	32.66	6
ATOM	2628	CD1	LEU A 330	28.051	53.904	56.022	1.00	31.74	6
ATOM	2629	CD2	LEU A 330	29.674	52.769	54.509	1.00	30.73	6
ATOM	2630	C	LEU A 330	28.877	55.631	51.428	1.00	37.28	6
ATOM	2631	O	LEU A 330	28.395	54.901	50.557	1.00	40.56	8
ATOM	2632	N	LYS A 331	28.806	56.957	51.383	1.00	38.24	7
ATOM	2633	CA	LYS A 331	28.140	57.661	50.294	1.00	39.59	6
ATOM	2634	CB	LYS A 331	27.994	59.146	50.643	1.00	42.31	6
ATOM	2635	CG	LYS A 331	27.129	59.399	51.873	1.00	45.93	6
ATOM	2636	CD	LYS A 331	27.017	60.879	52.244	1.00	49.72	6
ATOM	2637	CE	LYS A 331	26.271	61.698	51.193	1.00	53.66	6
ATOM	2638	NZ	LYS A 331	26.053	63.114	51.640	1.00	54.22	7
ATOM	2639	C	LYS A 331	28.863	57.514	48.958	1.00	41.02	6
ATOM	2640	O	LYS A 331	28.220	57.485	47.904	1.00	39.58	8

Figure 17-41

ATOM	2641	N	SER	A	332	30.192	57.413	49.005	1.00	42.69	7
ATOM	2642	CA	SER	A	332	30.998	57.274	47.792	1.00	46.02	6
ATOM	2643	CB	SER	A	332	32.494	57.243	48.124	1.00	47.51	6
ATOM	2644	OG	SER	A	332	32.862	56.066	48.823	1.00	50.97	8
ATOM	2645	C	SER	A	332	30.634	56.007	47.040	1.00	48.51	6
ATOM	2646	O	SER	A	332	30.706	55.959	45.811	1.00	49.45	8
ATOM	2647	N	ILE	A	333	30.241	54.982	47.786	1.00	51.56	7
ATOM	2648	CA	ILE	A	333	29.869	53.713	47.187	1.00	54.86	6
ATOM	2649	CB	ILE	A	333	29.657	52.626	48.246	1.00	55.80	6
ATOM	2650	CG2	ILE	A	333	29.388	51.285	47.559	1.00	52.34	6
ATOM	2651	CG1	ILE	A	333	30.892	52.522	49.140	1.00	56.89	6
ATOM	2652	CD1	ILE	A	333	30.766	51.456	50.204	1.00	60.31	6
ATOM	2653	C	ILE	A	333	28.579	53.813	46.396	1.00	57.07	6
ATOM	2654	O	ILE	A	333	27.572	54.321	46.897	1.00	55.59	8
ATOM	2655	N	ASP	A	334	28.623	53.320	45.160	1.00	61.14	7
ATOM	2656	CA	ASP	A	334	27.456	53.300	44.281	1.00	65.55	6
ATOM	2657	CB	ASP	A	334	27.888	53.259	42.811	1.00	69.19	6
ATOM	2658	CG	ASP	A	334	28.784	52.073	42.491	1.00	70.21	6
ATOM	2659	OD1	ASP	A	334	29.097	51.875	41.298	1.00	71.47	8
ATOM	2660	OD2	ASP	A	334	29.181	51.344	43.427	1.00	70.91	8
ATOM	2661	C	ASP	A	334	26.660	52.041	44.627	1.00	65.65	6
ATOM	2662	O	ASP	A	334	26.797	50.996	43.990	1.00	63.91	8
ATOM	2663	N	PHE	A	335	25.822	52.153	45.649	1.00	65.73	7
ATOM	2664	CA	PHE	A	335	25.041	51.021	46.104	1.00	63.44	6
ATOM	2665	CB	PHE	A	335	24.980	51.034	47.632	1.00	58.05	6
ATOM	2666	CG	PHE	A	335	24.039	50.028	48.195	1.00	53.82	6
ATOM	2667	CD1	PHE	A	335	24.178	48.679	47.886	1.00	52.40	6
ATOM	2668	CD2	PHE	A	335	22.978	50.429	48.989	1.00	51.33	6
ATOM	2669	CE1	PHE	A	335	23.265	47.742	48.356	1.00	52.73	6
ATOM	2670	CE2	PHE	A	335	22.062	49.503	49.462	1.00	53.20	6
ATOM	2671	CZ	PHE	A	335	22.204	48.151	49.144	1.00	51.76	6
ATOM	2672	C	PHE	A	335	23.629	50.893	45.535	1.00	65.55	6
ATOM	2673	O	PHE	A	335	23.230	49.810	45.097	1.00	67.33	8
ATOM	2674	N	GLU	A	336	22.874	51.986	45.537	1.00	66.47	7
ATOM	2675	CA	GLU	A	336	21.497	51.948	45.048	1.00	67.43	6
ATOM	2676	CB	GLU	A	336	21.422	51.379	43.626	1.00	71.79	6
ATOM	2677	CG	GLU	A	336	19.982	51.245	43.116	1.00	78.77	6
ATOM	2678	CD	GLU	A	336	19.868	50.505	41.789	1.00	82.67	6
ATOM	2679	OE1	GLU	A	336	20.232	49.306	41.734	1.00	83.29	8
ATOM	2680	OE2	GLU	A	336	19.410	51.126	40.801	1.00	84.26	8
ATOM	2681	C	GLU	A	336	20.655	51.069	45.971	1.00	64.72	6
ATOM	2682	O	GLU	A	336	20.686	49.840	45.876	1.00	59.84	8
ATOM	2683	N	GLU	A	337	19.901	51.710	46.858	1.00	64.47	7
ATOM	2684	CA	GLU	A	337	19.045	51.003	47.805	1.00	65.83	6
ATOM	2685	CB	GLU	A	337	18.398	52.003	48.759	1.00	64.20	6
ATOM	2686	CG	GLU	A	337	17.753	51.370	49.964	1.00	64.26	6
ATOM	2687	CD	GLU	A	337	18.774	50.600	50.850	1.00	64.04	6
ATOM	2688	OE1	GLU	A	337	19.741	51.322	51.261	1.00	61.66	8
ATOM	2689	OE2	GLU	A	337	18.608	49.483	51.132	1.00	63.64	8
ATOM	2690	C	GLU	A	337	17.950	50.239	47.063	1.00	67.13	6
ATOM	2691	O	GLU	A	337	17.269	50.807	46.205	1.00	68.27	8
ATOM	2692	N	PHE	A	338	17.779	48.960	47.394	1.00	67.22	7
ATOM	2693	CA	PHE	A	338	16.764	48.129	46.748	1.00	68.05	6
ATOM	2694	CB	PHE	A	338	16.445	46.919	47.626	1.00	69.68	6
ATOM	2695	CG	PHE	A	338	15.228	46.158	47.187	1.00	72.35	6
ATOM	2696	CD1	PHE	A	338	15.122	45.674	45.888	1.00	72.37	6
ATOM	2697	CD2	PHE	A	338	14.172	45.941	48.074	1.00	73.61	6
ATOM	2698	CE1	PHE	A	338	13.980	44.984	45.478	1.00	73.39	6
ATOM	2699	CE2	PHE	A	338	13.024	45.250	47.672	1.00	73.26	6
ATOM	2700	CZ	PHE	A	338	12.929	44.771	46.369	1.00	73.34	6
ATOM	2701	C	PHE	A	338	15.481	48.902	46.434	1.00	68.45	6
ATOM	2702	O	PHE	A	338	15.286	49.367	45.310	1.00	67.92	8
ATOM	2703	N	ASP	A	339	14.606	49.026	47.426	1.00	68.98	7
ATOM	2704	CA	ASP	A	339	13.358	49.759	47.261	1.00	70.68	6
ATOM	2705	CB	ASP	A	339	12.596	49.758	48.588	1.00	71.06	6
ATOM	2706	CG	ASP	A	339	11.381	50.678	48.581	1.00	72.05	6

ATOM	2707	OD1	ASP	A	339	11.548	51.893	48.320	1.00	72.29	8
ATOM	2708	OD2	ASP	A	339	10.262	50.188	48.858	1.00	71.03	8
ATOM	2709	C	ASP	A	339	13.715	51.183	46.853	1.00	73.18	6
ATOM	2710	O	ASP	A	339	14.407	51.884	47.592	1.00	73.78	8
ATOM	2711	N	ASP	A	340	13.247	51.600	45.677	1.00	76.36	7
ATOM	2712	CA	ASP	A	340	13.518	52.943	45.152	1.00	78.34	6
ATOM	2713	CB	ASP	A	340	12.410	53.385	44.189	1.00	77.55	6
ATOM	2714	CG	ASP	A	340	12.462	52.655	42.864	1.00	78.90	6
ATOM	2715	OD1	ASP	A	340	12.348	51.408	42.855	1.00	78.38	8
ATOM	2716	OD2	ASP	A	340	12.620	53.336	41.830	1.00	78.74	8
ATOM	2717	C	ASP	A	340	13.687	54.017	46.214	1.00	79.51	6
ATOM	2718	O	ASP	A	340	14.587	54.856	46.117	1.00	80.19	8
ATOM	2719	N	GLU	A	341	12.824	54.000	47.224	1.00	79.64	7
ATOM	2720	CA	GLU	A	341	12.922	54.998	48.271	1.00	80.05	6
ATOM	2721	CB	GLU	A	341	12.269	56.301	47.811	1.00	83.75	6
ATOM	2722	CG	GLU	A	341	12.411	57.442	48.806	1.00	89.02	6
ATOM	2723	CD	GLU	A	341	11.756	58.724	48.328	1.00	91.52	6
ATOM	2724	OE1	GLU	A	341	10.515	58.738	48.175	1.00	93.33	8
ATOM	2725	OE2	GLU	A	341	12.484	59.716	48.102	1.00	92.65	8
ATOM	2726	C	GLU	A	341	12.317	54.578	49.597	1.00	77.98	6
ATOM	2727	O	GLU	A	341	11.102	54.610	49.777	1.00	79.82	8
ATOM	2728	N	VAL	A	342	13.179	54.181	50.523	1.00	74.49	7
ATOM	2729	CA	VAL	A	342	12.745	53.793	51.859	1.00	71.55	6
ATOM	2730	CB	VAL	A	342	13.224	52.383	52.245	1.00	72.40	6
ATOM	2731	CG1	VAL	A	342	12.672	52.004	53.610	1.00	71.16	6
ATOM	2732	CG2	VAL	A	342	12.797	51.391	51.207	1.00	74.35	6
ATOM	2733	C	VAL	A	342	13.454	54.778	52.766	1.00	68.46	6
ATOM	2734	O	VAL	A	342	12.952	55.154	53.829	1.00	68.96	8
ATOM	2735	N	ASP	A	343	14.636	55.184	52.311	1.00	61.61	7
ATOM	2736	CA	ASP	A	343	15.486	56.114	53.029	1.00	54.91	6
ATOM	2737	CB	ASP	A	343	14.678	57.303	53.543	1.00	55.06	6
ATOM	2738	CG	ASP	A	343	15.556	58.390	54.114	1.00	54.44	6
ATOM	2739	OD1	ASP	A	343	15.002	59.351	54.694	1.00	56.20	8
ATOM	2740	OD2	ASP	A	343	16.795	58.287	53.969	1.00	49.32	8
ATOM	2741	C	ASP	A	343	16.152	55.401	54.198	1.00	50.85	6
ATOM	2742	O	ASP	A	343	15.557	55.209	55.257	1.00	49.32	8
ATOM	2743	N	ARG	A	344	17.396	55.004	53.980	1.00	47.84	7
ATOM	2744	CA	ARG	A	344	18.195	54.321	54.981	1.00	45.34	6
ATOM	2745	CB	ARG	A	344	18.883	53.099	54.358	1.00	45.00	6
ATOM	2746	CG	ARG	A	344	17.950	51.969	53.974	1.00	38.03	6
ATOM	2747	CD	ARG	A	344	17.185	51.531	55.188	1.00	35.83	6
ATOM	2748	NE	ARG	A	344	16.278	50.439	54.885	1.00	39.20	7
ATOM	2749	CZ	ARG	A	344	15.350	49.993	55.724	1.00	39.89	6
ATOM	2750	NH1	ARG	A	344	15.217	50.561	56.917	1.00	40.17	7
ATOM	2751	NH2	ARG	A	344	14.566	48.976	55.375	1.00	40.75	7
ATOM	2752	C	ARG	A	344	19.250	55.278	55.515	1.00	44.72	6
ATOM	2753	O	ARG	A	344	20.170	54.869	56.223	1.00	46.97	8
ATOM	2754	N	SER	A	345	19.113	56.552	55.157	1.00	45.81	7
ATOM	2755	CA	SER	A	345	20.045	57.596	55.577	1.00	43.66	6
ATOM	2756	CB	SER	A	345	19.538	58.960	55.115	1.00	43.44	6
ATOM	2757	CG	SER	A	345	18.292	59.260	55.722	1.00	45.62	8
ATOM	2758	C	SER	A	345	20.258	57.627	57.089	1.00	42.79	6
ATOM	2759	O	SER	A	345	21.364	57.902	57.552	1.00	42.62	8
ATOM	2760	N	TYR	A	346	19.200	57.354	57.851	1.00	40.55	7
ATOM	2761	CA	TYR	A	346	19.280	57.352	59.308	1.00	41.05	6
ATOM	2762	CB	TYR	A	346	17.971	56.819	59.905	1.00	41.74	6
ATOM	2763	CG	TYR	A	346	17.668	55.355	59.630	1.00	43.47	6
ATOM	2764	CD1	TYR	A	346	18.331	54.333	60.328	1.00	44.45	6
ATOM	2765	CE1	TYR	A	346	18.044	52.983	60.088	1.00	41.02	6
ATOM	2766	CD2	TYR	A	346	16.710	54.988	58.682	1.00	42.08	6
ATOM	2767	CE2	TYR	A	346	16.416	53.644	58.434	1.00	40.59	6
ATOM	2768	CZ	TYR	A	346	17.086	52.649	59.139	1.00	41.66	6
ATOM	2769	OH	TYR	A	346	16.806	51.324	58.884	1.00	39.60	8
ATOM	2770	C	TYR	A	346	20.466	56.517	59.796	1.00	42.92	6
ATOM	2771	O	TYR	A	346	21.101	56.844	60.799	1.00	42.65	8
ATOM	2772	N	MET	A	347	20.757	55.443	59.067	1.00	44.59	7

Figure 17-43

ATOM	2773	CA	MET	A	347	21.859	54.546	59.388	1.00	45.89	6
ATOM	2774	CB	MET	A	347	21.950	53.433	58.353	1.00	45.51	6
ATOM	2775	CG	MET	A	347	20.727	52.567	58.244	1.00	45.01	6
ATOM	2776	SD	MET	A	347	21.062	51.258	57.066	1.00	47.13	16
ATOM	2777	CE	MET	A	347	21.545	52.237	55.676	1.00	44.55	6
ATOM	2778	C	MET	A	347	23.188	55.286	59.404	1.00	48.47	6
ATOM	2779	O	MET	A	347	24.129	54.888	60.098	1.00	49.49	8
ATOM	2780	N	LEU	A	348	23.259	56.351	58.610	1.00	49.03	7
ATOM	2781	CA	LEU	A	348	24.458	57.178	58.499	1.00	48.86	6
ATOM	2782	CB	LEU	A	348	24.355	56.082	57.269	1.00	45.51	6
ATOM	2783	CG	LEU	A	348	24.280	57.424	55.895	1.00	44.47	6
ATOM	2784	CD1	LEU	A	348	23.908	58.476	54.859	1.00	43.62	6
ATOM	2785	CD2	LEU	A	348	25.618	56.757	55.565	1.00	42.53	6
ATOM	2786	C	LEU	A	348	24.644	58.049	59.738	1.00	49.33	6
ATOM	2787	O	LEU	A	348	25.765	58.369	60.123	1.00	49.78	8
ATOM	2788	N	GLU	A	349	23.537	58.428	60.358	1.00	48.34	7
ATOM	2789	CA	GLU	A	349	23.591	59.279	61.533	1.00	49.24	6
ATOM	2790	CB	GLU	A	349	22.198	59.848	61.811	1.00	48.36	6
ATOM	2791	CG	GLU	A	349	21.628	60.584	60.607	1.00	45.52	6
ATOM	2792	CD	GLU	A	349	22.598	61.619	60.065	1.00	42.94	6
ATOM	2793	OE1	GLU	A	349	22.934	62.560	60.812	1.00	40.82	8
ATOM	2794	OE2	GLU	A	349	23.028	61.483	58.900	1.00	38.30	8
ATOM	2795	C	GLU	A	349	24.119	58.531	62.745	1.00	48.32	6
ATOM	2796	O	GLU	A	349	25.226	58.783	63.219	1.00	47.87	8
ATOM	2797	N	THR	A	350	23.325	57.602	63.248	1.00	48.97	7
ATOM	2798	CA	THR	A	350	23.744	56.832	64.398	1.00	50.70	6
ATOM	2799	CB	THR	A	350	22.558	56.596	65.342	1.00	51.02	6
ATOM	2800	OG1	THR	A	350	22.071	57.865	65.803	1.00	49.11	8
ATOM	2801	CG2	THR	A	350	22.983	55.763	66.537	1.00	51.58	6
ATOM	2802	C	THR	A	350	24.361	55.507	63.954	1.00	49.56	6
ATOM	2803	O	THR	A	350	23.979	54.947	62.923	1.00	50.55	8
ATOM	2804	N	LEU	A	351	25.333	55.028	64.725	1.00	46.88	7
ATOM	2805	CA	LEU	A	351	26.018	53.781	64.417	1.00	45.35	6
ATOM	2806	CB	LEU	A	351	27.342	53.726	65.185	1.00	47.05	6
ATOM	2807	CG	LEU	A	351	28.257	52.502	65.072	1.00	49.54	6
ATOM	2808	CD1	LEU	A	351	29.575	52.777	65.766	1.00	51.50	6
ATOM	2809	CD2	LEU	A	351	27.603	51.302	65.692	1.00	48.35	6
ATOM	2810	C	LEU	A	351	25.145	52.584	64.772	1.00	44.79	6
ATOM	2811	O	LEU	A	351	25.131	51.578	64.061	1.00	41.45	8
ATOM	2812	N	LYS	A	352	24.420	52.711	65.880	1.00	45.27	7
ATOM	2813	CA	LYS	A	352	23.531	51.662	66.375	1.00	44.62	6
ATOM	2814	CB	LYS	A	352	23.764	51.464	67.873	1.00	42.23	6
ATOM	2815	CG	LYS	A	352	25.197	51.075	68.187	1.00	44.94	6
ATOM	2816	CD	LYS	A	352	25.572	51.262	69.650	1.00	46.80	6
ATOM	2817	CE	LYS	A	352	24.765	50.389	70.581	1.00	45.79	6
ATOM	2818	NZ	LYS	A	352	25.236	50.586	71.975	1.00	47.31	7
ATOM	2819	C	LYS	A	352	22.096	52.087	66.116	1.00	45.12	6
ATOM	2820	O	LYS	A	352	21.837	53.236	65.756	1.00	47.07	8
ATOM	2821	N	ASP	A	353	21.162	51.161	66.285	1.00	44.62	7
ATOM	2822	CA	ASP	A	353	19.761	51.474	66.060	1.00	46.43	6
ATOM	2823	CB	ASP	A	353	19.302	50.943	64.692	1.00	49.38	6
ATOM	2824	CG	ASP	A	353	19.813	49.546	64.396	1.00	51.52	6
ATOM	2825	OD1	ASP	A	353	21.028	49.396	64.158	1.00	55.36	8
ATOM	2826	OD2	ASP	A	353	19.005	48.596	64.398	1.00	52.35	8
ATOM	2827	C	ASP	A	353	18.841	50.968	67.165	1.00	45.90	6
ATOM	2828	O	ASP	A	353	19.152	50.001	67.854	1.00	45.98	8
ATOM	2829	N	PRO	A	354	17.687	51.629	67.348	1.00	45.86	7
ATOM	2830	CD	PRO	A	354	17.162	52.775	66.587	1.00	45.36	6
ATOM	2831	CA	PRO	A	354	16.723	51.243	68.378	1.00	45.52	6
ATOM	2832	CB	PRO	A	354	15.585	52.245	68.159	1.00	44.77	6
ATOM	2833	CG	PRO	A	354	15.681	52.513	66.664	1.00	45.06	6
ATOM	2834	C	PRO	A	354	16.277	49.804	68.188	1.00	44.13	6
ATOM	2835	O	PRO	A	354	16.352	49.271	67.078	1.00	42.90	8
ATOM	2836	N	TRP	A	355	15.821	49.174	69.267	1.00	42.77	7
ATOM	2837	CA	TRP	A	355	15.358	47.801	69.168	1.00	43.35	6
ATOM	2838	CB	TRP	A	355	14.982	47.225	70.539	1.00	47.11	6

ATOM	2839	CG	TRP	A	355	16.168	46.752	71.322	1.00	52.43	6
ATOM	2840	CD2	TRP	A	355	16.574	45.391	71.519	1.00	53.15	6
ATOM	2841	CE2	TRP	A	355	17.789	45.416	72.238	1.00	54.97	6
ATOM	2842	CE3	TRP	A	355	16.031	44.153	71.155	1.00	53.39	6
ATOM	2843	CD1	TRP	A	355	17.125	47.526	71.916	1.00	54.39	6
ATOM	2844	NE1	TRP	A	355	18.103	46.731	72.468	1.00	57.31	7
ATOM	2845	CZ2	TRP	A	355	18.469	44.249	72.602	1.00	54.97	6
ATOM	2846	CZ3	TRP	A	355	16.706	42.995	71.518	1.00	55.77	6
ATOM	2847	CH2	TRP	A	355	17.913	43.052	72.234	1.00	54.84	6
ATOM	2848	C	TRP	A	355	14.177	47.690	68.230	1.00	41.94	6
ATOM	2849	O	TRP	A	355	13.508	48.677	67.915	1.00	41.39	8
ATOM	2850	N	ARG	A	356	13.942	46.471	67.775	1.00	38.60	7
ATOM	2851	CA	ARG	A	356	12.855	46.185	66.866	1.00	36.55	6
ATOM	2852	CB	ARG	A	356	13.413	46.044	65.451	1.00	35.06	6
ATOM	2853	CG	ARG	A	356	14.120	47.308	64.976	1.00	32.47	6
ATOM	2854	CD	ARG	A	356	14.969	47.082	63.733	1.00	29.54	6
ATOM	2855	NE	ARG	A	356	15.600	48.323	63.296	1.00	28.91	7
ATOM	2856	CZ	ARG	A	356	16.514	48.403	62.335	1.00	30.60	6
ATOM	2857	NH1	ARG	A	356	16.916	47.305	61.702	1.00	33.52	7
ATOM	2858	NH2	ARG	A	356	17.020	49.582	61.996	1.00	30.10	7
ATOM	2859	C	ARG	A	356	12.270	44.879	67.361	1.00	36.01	6
ATOM	2860	O	ARG	A	356	12.447	43.831	66.742	1.00	38.38	8
ATOM	2861	N	GLY	A	357	11.587	44.949	68.499	1.00	36.04	7
ATOM	2862	CA	GLY	A	357	11.001	43.758	69.085	1.00	36.08	6
ATOM	2863	C	GLY	A	357	9.514	43.596	68.851	1.00	34.51	6
ATOM	2864	O	GLY	A	357	8.943	44.196	67.943	1.00	36.77	8
ATOM	2865	N	GLY	A	358	8.892	42.772	69.687	1.00	36.04	7
ATOM	2866	CA	GLY	A	358	7.466	42.506	69.593	1.00	32.26	6
ATOM	2867	C	GLY	A	358	7.106	41.263	70.385	1.00	29.85	6
ATOM	2868	O	GLY	A	358	7.832	40.839	71.288	1.00	28.86	8
ATOM	2869	N	GLU	A	359	5.975	40.667	70.055	1.00	30.88	7
ATOM	2870	CA	GLU	A	359	5.550	39.455	70.743	1.00	32.58	6
ATOM	2871	CB	GLU	A	359	4.034	39.289	70.604	1.00	38.60	6
ATOM	2872	CG	GLU	A	359	3.230	40.435	71.222	1.00	47.44	6
ATOM	2873	CD	GLU	A	359	1.957	40.762	70.445	1.00	50.93	6
ATOM	2874	OE1	GLU	A	359	1.123	39.852	70.221	1.00	52.13	8
ATOM	2875	OE2	GLU	A	359	1.798	41.942	70.061	1.00	51.03	8
ATOM	2876	C	GLU	A	359	6.250	38.275	70.091	1.00	28.29	6
ATOM	2877	O	GLU	A	359	6.790	38.382	68.997	1.00	27.88	8
ATOM	2878	N	VAL	A	360	6.263	37.147	70.772	1.00	27.97	7
ATOM	2879	CA	VAL	A	360	6.859	35.957	70.193	1.00	25.86	6
ATOM	2880	CB	VAL	A	360	7.673	35.168	71.237	1.00	22.02	6
ATOM	2881	CG1	VAL	A	360	8.155	33.849	70.641	1.00	19.45	6
ATOM	2882	CG2	VAL	A	360	8.850	36.009	71.698	1.00	17.88	6
ATOM	2883	C	VAL	A	360	5.703	35.099	69.670	1.00	28.04	6
ATOM	2884	C	VAL	A	360	4.842	34.655	70.440	1.00	27.34	8
ATOM	2885	N	ARG	A	361	5.663	34.898	68.358	1.00	27.70	7
ATOM	2886	C..	ARG	A	361	4.612	34.091	67.765	1.00	32.85	6
ATOM	2887	CB	ARG	A	361	4.693	34.164	66.242	1.00	32.30	6
ATOM	2888	CG	ARG	A	361	4.243	35.504	65.687	1.00	38.81	6
ATOM	2889	CD	ARG	A	361	4.546	35.653	64.201	1.00	40.09	6
ATOM	2890	NE	ARG	A	361	5.974	35.812	63.961	1.00	38.77	7
ATOM	2891	CZ	ARG	A	361	6.514	35.989	62.763	1.00	39.21	6
ATOM	2892	NH1	ARG	A	361	5.748	36.027	61.685	1.00	40.79	7
ATOM	2893	NH2	ARG	A	361	7.822	36.145	62.643	1.00	42.94	7
ATOM	2894	C	ARG	A	361	4.689	32.638	68.222	1.00	35.65	6
ATOM	2895	O	ARG	A	361	5.768	32.097	68.471	1.00	37.08	8
ATOM	2896	N	LYS	A	362	3.526	32.017	68.347	1.00	37.80	7
ATOM	2897	CA	LYS	A	362	3.436	30.626	68.757	1.00	39.91	6
ATOM	2898	CB	LYS	A	362	1.982	30.152	68.648	1.00	43.43	6
ATOM	2899	CG	LYS	A	362	1.014	30.803	69.640	1.00	45.11	6
ATOM	2900	CD	LYS	A	362	1.117	32.346	69.673	1.00	49.43	6
ATOM	2901	CE	LYS	A	362	0.813	33.022	68.327	1.00	45.02	6
ATOM	2902	NZ	LYS	A	362	0.962	34.509	68.422	1.00	41.08	7
ATOM	2903	C	LYS	A	362	4.320	29.809	67.831	1.00	39.25	6
ATOM	2904	O	LYS	A	362	4.953	28.835	68.248	1.00	35.45	8

ATOM	2905	N	GLU A 363	4.358	30.229	66.568	1.00	41.13	7
ATOM	2906	CA	GLU A 363	5.147	29.554	65.539	1.00	43.96	6
ATOM	2907	CB	GLU A 363	5.225	30.416	64.278	1.00	45.90	6
ATOM	2908	CG	GLU A 363	3.892	30.876	63.741	1.00	50.68	6
ATOM	2909	CD	GLU A 363	4.045	31.738	62.507	1.00	54.11	6
ATOM	2910	OE1	GLU A 363	4.571	31.224	61.494	1.00	53.90	8
ATOM	2911	OE2	GLU A 363	3.648	32.927	62.552	1.00	56.05	8
ATOM	2912	C	GLU A 363	6.558	29.296	66.046	1.00	42.39	6
ATOM	2913	O	GLU A 363	7.062	28.169	65.989	1.00	41.48	8
ATOM	2914	N	VAL A 364	7.183	30.360	66.540	1.00	37.27	7
ATOM	2915	CA	VAL A 364	8.535	30.291	67.064	1.00	35.30	6
ATOM	2916	CB	VAL A 364	9.038	31.696	67.469	1.00	36.88	6
ATOM	2917	CG1	VAL A 364	10.444	31.599	68.043	1.00	37.77	6
ATOM	2918	CG2	VAL A 364	9.018	32.628	66.252	1.00	34.78	6
ATOM	2919	C	VAL A 364	8.650	29.361	68.268	1.00	33.01	6
ATOM	2920	O	VAL A 364	9.622	28.614	68.379	1.00	31.55	8
ATOM	2921	N	LYS A 365	7.664	29.409	69.165	1.00	32.61	7
ATOM	2922	CA	LYS A 365	7.674	28.567	70.362	1.00	30.96	6
ATOM	2923	CB	LYS A 365	6.598	29.010	71.358	1.00	30.13	6
ATOM	2924	CG	LYS A 365	6.826	30.409	71.899	1.00	36.02	6
ATOM	2925	CD	LYS A 365	5.837	30.781	72.995	1.00	38.94	6
ATOM	2926	CE	LYS A 365	6.120	32.187	73.509	1.00	41.58	6
ATOM	2927	NZ	LYS A 365	5.191	32.611	74.585	1.00	44.29	7
ATOM	2928	C	LYS A 365	7.452	27.114	70.007	1.00	30.32	6
ATOM	2929	O	LYS A 365	8.195	26.237	70.442	1.00	31.32	8
ATOM	2930	N	ASP A 366	6.427	26.863	69.209	1.00	29.85	7
ATOM	2931	CA	ASP A 366	6.115	25.509	68.807	1.00	32.07	6
ATOM	2932	CB	ASP A 366	4.948	25.522	67.818	1.00	35.98	6
ATOM	2933	CG	ASP A 366	3.711	26.206	68.381	1.00	39.88	6
ATOM	2934	OD1	ASP A 366	3.124	25.692	69.359	1.00	40.16	8
ATOM	2935	OD2	ASP A 366	3.326	27.266	67.848	1.00	43.21	8
ATOM	2936	C	ASP A 366	7.343	24.866	68.161	1.00	33.07	6
ATOM	2937	O	ASP A 366	7.753	23.763	68.540	1.00	32.64	8
ATOM	2938	N	THR A 367	7.932	25.565	67.193	1.00	31.89	7
ATOM	2939	CA	THR A 367	9.088	25.045	66.490	1.00	31.17	6
ATOM	2940	CB	THR A 367	9.712	26.070	65.572	1.00	31.55	6
ATOM	2941	OG1	THR A 367	8.707	26.620	64.714	1.00	34.37	8
ATOM	2942	CG2	THR A 367	10.780	25.404	64.723	1.00	33.55	6
ATOM	2943	C	THR A 367	10.146	24.633	67.472	1.00	33.09	6
ATOM	2944	O	THR A 367	10.586	23.476	67.485	1.00	38.62	8
ATOM	2945	N	LEU A 368	10.570	25.579	68.298	1.00	31.85	7
ATOM	2946	CA	LEU A 368	11.582	25.264	69.288	1.00	32.87	6
ATOM	2947	CB	LEU A 368	11.848	26.478	70.179	1.00	27.73	6
ATOM	2948	CG	LEU A 368	12.887	27.449	69.588	1.00	29.05	6
ATOM	2949	CD1	LEU A 368	14.260	26.777	69.541	1.00	23.05	6
ATOM	2950	CD2	LEU A 368	12.473	27.896	68.193	1.00	26.53	6
ATOM	2951	C	LEU A 368	11.157	24.053	70.107	1.00	35.16	6
ATOM	2952	O	LEU A 368	11.910	23.077	70.217	1.00	35.18	8
ATOM	2953	N	GLU A 369	9.942	24.101	70.649	1.00	37.56	7
ATOM	2954	CA	GLU A 369	9.431	22.993	71.442	1.00	40.23	6
ATOM	2955	CB	GLU A 369	7.956	23.216	71.770	1.00	42.07	6
ATOM	2956	CG	GLU A 369	7.722	24.460	72.617	1.00	48.51	6
ATOM	2957	CD	GLU A 369	6.281	24.616	73.067	1.00	51.93	6
ATOM	2958	OE1	GLU A 369	5.777	23.724	73.782	1.00	52.84	8
ATOM	2959	OE2	GLU A 369	5.652	25.636	72.710	1.00	58.33	8
ATOM	2960	C	GLU A 369	9.633	21.672	70.701	1.00	41.14	6
ATOM	2961	O	GLU A 369	10.087	20.684	71.286	1.00	41.87	8
ATOM	2962	N	LYS A 370	9.309	21.653	69.411	1.00	39.65	7
ATOM	2963	CA	LYS A 370	9.497	20.443	68.636	1.00	38.26	6
ATOM	2964	CB	LYS A 370	9.144	20.654	67.166	1.00	40.63	6
ATOM	2965	CG	LYS A 370	7.675	20.597	66.854	1.00	44.49	6
ATOM	2966	CD	LYS A 370	7.495	20.358	65.363	1.00	49.95	6
ATOM	2967	CE	LYS A 370	6.052	20.023	65.015	1.00	54.28	6
ATOM	2968	NZ	LYS A 370	5.890	19.679	63.574	1.00	55.44	7
ATOM	2969	C	LYS A 370	10.948	20.034	68.730	1.00	37.85	6
ATOM	2970	O	LYS A 370	11.261	18.930	69.156	1.00	37.95	8

ATOM	2971	N	ALA A	371	11.827	20.944	68.325	1.00	37.78	7
ATOM	2972	CA	ALA A	371	13.264	20.704	68.340	1.00	36.39	6
ATOM	2973	CB	ALA A	371	14.007	22.030	68.200	1.00	37.73	6
ATOM	2974	C	ALA A	371	13.719	19.972	69.603	1.00	35.42	6
ATOM	2975	O	ALA A	371	14.424	18.964	69.525	1.00	32.06	8
ATOM	2976	N	ALA A	372	13.317	20.478	70.766	1.00	33.96	7
ATOM	2977	CA	ALA A	372	13.695	19.848	72.024	1.00	32.22	6
ATOM	2978	CB	ALA A	372	12.946	20.486	73.165	1.00	28.27	6
ATOM	2979	C	ALA A	372	13.372	18.362	71.953	1.00	31.75	6
ATOM	2980	O	ALA A	372	14.183	17.517	72.338	1.00	31.56	8
ATOM	2981	N	ALA A	373	12.187	18.059	71.432	1.00	32.72	7
ATOM	2982	CA	ALA A	373	11.710	16.684	71.305	1.00	32.32	6
ATOM	2983	CB	ALA A	373	10.206	16.689	71.103	1.00	30.18	6
ATOM	2984	C	ALA A	373	12.385	15.921	70.172	1.00	33.13	6
ATOM	2985	OT1	ALA A	373	13.078	14.926	70.468	1.00	35.87	8
ATOM	2986	OT2	ALA A	373	12.218	16.320	69.003	1.00	34.11	8
ATOM	2987	ZN	ZN Z	951	22.693	34.497	53.990	1.00	36.45	6
ATOM	2988	OH2	WAT S	1	35.654	44.211	49.416	1.00	9.27	8
ATOM	2989	OH2	WAT S	2	24.480	33.130	53.069	1.00	21.27	8
ATOM	2990	OH2	WAT S	3	22.124	30.277	59.314	1.00	14.69	8
ATOM	2991	OH2	WAT S	4	13.839	20.611	75.741	1.00	27.94	8
ATOM	2992	OH2	WAT S	5	34.033	41.903	46.522	1.00	44.54	8
ATOM	2993	OH2	WAT S	6	15.039	42.130	55.781	1.00	23.79	8
ATOM	2994	OH2	WAT S	7	32.737	41.397	75.900	1.00	15.80	8
ATOM	2995	OH2	WAT S	8	11.367	22.606	58.814	1.00	23.37	8
ATOM	2996	OH2	WAT S	9	13.909	18.160	65.105	1.00	29.93	8
ATOM	2997	OH2	WAT S	10	29.655	56.108	58.029	1.00	50.54	8
ATOM	2998	OH2	WAT S	11	45.405	17.964	51.885	1.00	9.28	8
ATOM	2999	OH2	WAT S	12	21.870	35.873	34.515	1.00	32.78	8
ATOM	3000	OH2	WAT S	13	43.504	35.670	33.779	1.00	28.85	8
ATOM	3001	OH2	WAT S	14	2.054	37.997	68.430	1.00	40.53	8
ATOM	3002	OH2	WAT S	15	49.730	28.024	55.966	1.00	21.42	8
ATOM	3003	OH2	WAT S	16	47.503	32.289	34.336	1.00	26.13	8
ATOM	3004	OH2	WAT S	17	6.101	26.102	64.434	1.00	21.69	8
ATOM	3005	OH2	WAT S	18	10.761	46.748	45.836	1.00	15.79	8
ATOM	3006	OH2	WAT S	19	9.146	16.861	61.441	1.00	16.68	8
ATOM	3007	OH2	WAT S	20	5.684	34.080	76.599	1.00	37.53	8
ATOM	3008	OH2	WAT S	21	14.896	33.163	49.117	1.00	34.17	8
ATOM	3009	OH2	WAT S	22	43.346	40.839	36.825	1.00	35.64	8
ATOM	3010	OH2	WAT S	23	0.516	27.705	69.174	1.00	21.02	8
ATOM	3011	OH2	WAT S	24	41.270	25.444	29.717	1.00	29.80	8
ATOM	3012	OH2	WAT S	25	17.818	29.142	54.584	1.00	27.92	8
ATOM	3013	OH2	WAT S	26	21.512	60.572	56.912	1.00	16.77	8
ATOM	3014	OH2	WAT S	27	21.211	33.582	48.347	1.00	23.93	8
ATOM	3015	OH2	WAT S	28	47.805	24.638	56.619	1.00	23.73	8
ATOM	3016	OH2	WAT S	29	44.624	50.302	58.154	1.00	16.79	8
ATOM	3017	OH2	WAT S	30	31.096	16.437	51.311	1.00	26.61	8
ATOM	3018	OH2	WAT S	31	39.837	38.833	55.145	1.00	32.28	8
ATOM	3019	OH2	WAT S	32	11.660	43.601	63.704	1.00	22.94	8
ATOM	3020	OH2	WAT S	33	49.899	23.474	53.058	1.00	26.85	8
ATOM	3021	OH2	WAT S	34	34.624	17.734	32.228	1.00	21.18	8
ATOM	3022	OH2	WAT S	35	26.926	15.913	62.444	1.00	27.01	8
ATOM	3023	OH2	WAT S	36	8.893	28.686	63.905	1.00	27.68	8
ATOM	3024	OH2	WAT S	37	23.381	26.634	43.532	1.00	24.42	8
ATOM	3025	OH2	WAT S	38	48.484	27.990	65.270	1.00	34.86	8
ATOM	3026	OH2	WAT S	39	43.382	28.410	74.379	1.00	25.68	8
ATOM	3027	OH2	WAT S	40	42.904	18.967	70.272	1.00	29.45	8
ATOM	3028	OH2	WAT S	41	20.521	53.828	50.298	1.00	22.35	8
ATOM	3029	OH2	WAT S	42	13.310	38.921	48.404	1.00	23.32	8
ATOM	3030	OH2	WAT S	43	9.787	46.265	60.012	1.00	33.51	8
ATOM	3031	OH2	WAT S	44	36.089	30.416	51.377	1.00	47.75	8
ATOM	3032	OH2	WAT S	45	14.831	48.131	42.151	1.00	50.96	8
ATOM	3033	OH2	WAT S	46	54.162	48.194	60.971	1.00	22.66	8
ATOM	3034	OH2	WAT S	47	38.943	61.290	63.509	1.00	33.73	8
ATOM	3035	OH2	WAT S	48	29.980	18.112	33.130	1.00	35.80	8
ATOM	3036	OH2	WAT S	49	31.879	50.673	44.528	1.00	24.39	8

114/263

Figure 17-47

ATOM	3037	OH2	WAT	S	50	39.863	14.629	64.307	1.00	24.19	8
ATOM	3038	OH2	WAT	S	51	26.119	29.471	38.549	1.00	27.78	8
ATOM	3039	OH2	WAT	S	52	48.070	41.589	44.011	1.00	36.38	8
ATOM	3040	OH2	WAT	S	53	50.802	29.649	52.495	1.00	31.04	8
ATOM	3041	OH2	WAT	S	54	49.540	35.532	71.585	1.00	20.96	8
ATOM	3042	OH2	WAT	S	55	6.887	23.426	64.961	1.00	17.49	8
ATOM	3043	OH2	WAT	S	56	25.698	39.891	37.674	1.00	51.51	8
ATOM	3044	OH2	WAT	S	57	45.498	44.101	55.393	1.00	37.34	8
ATOM	3045	OH2	WAT	S	58	44.661	34.733	46.902	1.00	44.52	8
ATOM	3046	OH2	WAT	S	59	21.912	21.320	79.233	1.00	26.96	8
ATOM	3047	OH2	WAT	S	60	27.290	21.016	77.320	1.00	27.74	8
ATOM	3048	OH2	WAT	S	61	19.809	49.810	61.716	1.00	46.14	8
ATOM	3049	OH2	WAT	S	62	30.843	18.035	41.441	1.00	42.23	8
ATOM	3050	OH2	WAT	S	63	19.055	33.379	60.511	1.00	28.99	8
ATOM	3051	OH2	WAT	S	64	47.925	33.253	61.470	1.00	34.93	8
ATOM	3052	OH2	WAT	S	65	32.500	36.000	41.000	1.00	35.33	8
ATOM	3053	OH2	WAT	S	66	27.245	56.551	44.579	1.00	34.19	8
ATOM	3054	OH2	WAT	S	67	5.176	32.914	54.669	1.00	41.89	8
ATOM	3055	OH2	WAT	S	68	41.159	51.018	49.348	1.00	27.31	8
ATOM	3056	OH2	WAT	S	69	12.869	50.298	61.877	1.00	31.30	8
ATOM	3057	OH2	WAT	S	70	17.499	12.826	63.854	1.00	24.91	8
ATOM	3058	OH2	WAT	S	71	27.152	12.189	53.999	1.00	18.76	8
ATOM	3059	OH2	WAT	S	72	25.213	54.809	67.866	1.00	61.35	8
ATOM	3060	OH2	WAT	S	73	17.671	48.515	53.188	1.00	37.63	8
ATOM	3061	OH2	WAT	S	74	23.765	60.846	66.579	1.00	21.81	8
ATOM	3062	OH2	WAT	S	75	35.535	27.040	70.698	1.00	34.04	8
ATOM	3063	OH2	WAT	S	76	26.280	16.065	76.564	1.00	32.20	8
ATOM	3064	OH2	WAT	S	77	18.451	25.555	45.150	1.00	28.55	8
ATOM	3065	OH2	WAT	S	78	10.446	61.273	48.633	1.00	44.74	8
ATOM	3066	OH2	WAT	S	79	13.256	24.051	73.017	1.00	35.45	8
ATOM	3067	OH2	WAT	S	80	23.571	13.292	69.937	1.00	49.49	8
ATOM	3068	OH2	WAT	S	81	29.891	18.071	46.109	1.00	22.84	8
ATOM	3069	OH2	WAT	S	82	12.886	42.723	75.807	1.00	35.31	8
ATOM	3070	OH2	WAT	S	83	41.348	15.471	45.004	1.00	47.24	8
ATOM	3071	OH2	WAT	S	84	13.406	44.647	71.349	1.00	49.67	8
ATOM	3072	OH2	WAT	S	85	30.444	35.217	51.882	1.00	38.15	8
ATOM	3073	OH2	WAT	S	86	5.217	40.817	61.244	1.00	19.51	8
ATOM	3074	OH2	WAT	S	87	8.891	21.532	56.838	1.00	30.72	8
ATOM	3075	OH2	WAT	S	88	41.816	25.022	72.452	1.00	22.92	8
ATOM	3076	OH2	WAT	S	89	50.621	36.644	60.248	1.00	29.29	8
ATOM	3077	OH2	WAT	S	90	26.008	34.532	49.627	1.00	45.42	8
ATOM	3078	OH2	WAT	S	91	8.131	39.168	54.903	1.00	31.50	8
ATOM	3079	OH2	WAT	S	92	16.591	58.091	57.551	1.00	34.73	8
ATOM	3080	OH2	WAT	S	93	34.773	54.065	69.382	1.00	36.05	8
ATOM	3081	OH2	WAT	S	94	42.105	31.720	71.257	1.00	35.49	8
ATOM	3082	OH2	WAT	S	95	29.684	52.077	73.172	1.00	35.17	8
ATOM	3083	OH2	WAT	S	96	26.411	37.426	38.934	1.00	41.68	8
ATOM	3084	OH2	WAT	S	97	41.183	52.989	62.927	1.00	50.77	8
ATOM	3085	OH2	WAT	S	98	21.167	6.202	63.102	1.00	33.36	8
ATOM	3086	OH2	WAT	S	99	25.060	18.985	36.669	1.00	46.63	8
ATOM	3087	OH2	WAT	S	100	37.304	39.027	73.722	1.00	25.99	8
ATOM	3088	OH2	WAT	S	101	15.911	54.635	39.343	1.00	29.88	8
ATOM	3089	OH2	WAT	S	102	48.730	25.803	59.572	1.00	37.97	8
ATOM	3090	OH2	WAT	S	103	24.029	42.997	74.111	1.00	25.23	8
ATOM	3091	OH2	WAT	S	104	42.477	21.773	46.986	1.00	49.05	8
ATOM	3092	OH2	WAT	S	105	29.984	22.945	31.397	1.00	44.21	8
ATOM	3093	OH2	WAT	S	106	40.850	36.936	31.885	1.00	43.26	8
ATOM	3094	OH2	WAT	S	107	9.750	32.487	48.823	1.00	35.71	8
ATOM	3095	OH2	WAT	S	108	7.618	30.171	58.896	1.00	40.03	8
ATOM	3096	OH2	WAT	S	109	17.603	13.771	59.767	1.00	50.33	8
ATOM	3097	OH2	WAT	S	110	22.590	8.744	67.501	1.00	34.81	8
ATOM	3098	OH2	WAT	S	111	21.034	29.771	76.056	1.00	30.02	8
ATOM	3099	OH2	WAT	S	112	24.791	14.674	50.081	1.00	51.96	8
ATOM	3100	OH2	WAT	S	113	40.750	47.494	54.056	1.00	46.98	8
ATOM	3101	OH2	WAT	S	114	7.708	42.479	58.027	1.00	34.08	8
ATOM	3102	OH2	WAT	S	115	32.375	49.136	77.566	1.00	27.53	8

Figure 17-48

ATOM	3103	OH2	WAT	S	116	5.596	17.009	64.551	1.00	39.15	8
ATOM	3104	OH2	WAT	S	117	20.194	50.998	70.563	1.00	19.73	8
ATOM	3105	OH2	WAT	S	118	23.853	64.927	64.164	1.00	27.16	8
ATOM	3106	OH2	WAT	S	119	9.277	43.601	46.279	1.00	32.31	8
ATOM	3107	OH2	WAT	S	120	15.613	24.398	46.723	1.00	55.20	8
ATOM	3108	OH2	WAT	S	121	33.110	16.122	54.229	1.00	35.91	8
ATOM	3109	OH2	WAT	S	122	26.772	34.085	33.852	1.00	37.49	8
ATOM	3110	OH2	WAT	S	123	28.654	37.783	75.829	1.00	47.30	8
ATOM	3111	OH2	WAT	S	124	49.180	22.653	59.678	1.00	37.33	8
ATOM	3112	OH2	WAT	S	125	20.561	27.788	65.975	1.00	67.86	8
ATOM	3113	OH2	WAT	S	126	34.251	13.344	57.366	1.00	36.18	8
ATOM	3114	OH2	WAT	S	127	49.215	36.854	48.117	1.00	33.63	8
ATOM	3115	OH2	WAT	S	128	45.826	19.588	41.601	1.00	44.07	8
ATOM	3116	OH2	WAT	S	129	18.693	56.382	64.014	1.00	47.77	8
ATOM	3117	OH2	WAT	S	130	44.181	24.202	36.963	1.00	32.70	8
ATOM	3118	OH2	WAT	S	131	19.160	51.901	38.133	1.00	54.07	8
ATOM	3119	OH2	WAT	S	132	16.904	36.558	48.679	1.00	42.21	8
ATOM	3120	OH2	WAT	S	133	46.851	26.029	34.353	1.00	56.33	8
ATOM	3121	OH2	WAT	S	134	3.925	41.533	68.647	1.00	45.99	8
ATOM	3122	OH2	WAT	S	135	44.590	38.382	78.167	1.00	44.50	8
ATOM	3123	OH2	WAT	S	136	6.384	19.317	71.166	1.00	28.17	8
ATOM	3124	OH2	WAT	S	137	17.982	39.823	66.487	1.00	49.31	8
ATOM	3125	OH2	WAT	S	138	8.317	22.286	61.863	1.00	43.42	8
ATOM	3126	OH2	WAT	S	139	29.248	14.196	55.622	1.00	35.55	8
ATOM	3127	OH2	WAT	S	140	30.377	33.180	80.320	1.00	43.94	8
ATOM	3128	OH2	WAT	S	141	41.842	32.906	27.392	1.00	24.82	8
ATOM	3129	OH2	WAT	S	142	33.971	3.859	64.002	1.00	41.93	8
ATOM	3130	OH2	WAT	S	143	27.314	8.087	70.916	1.00	49.03	8
ATOM	3131	OH2	WAT	S	144	4.310	39.006	64.550	1.00	32.70	8
ATOM	3132	OH2	WAT	S	145	2.940	19.950	63.265	1.00	33.24	8
ATOM	3133	OH2	WAT	S	146	24.134	47.625	60.121	1.00	44.24	8
ATOM	3134	OH2	WAT	S	147	25.035	53.746	42.337	1.00	47.82	8
ATOM	3135	OH2	WAT	S	148	32.767	38.897	49.651	1.00	21.86	8
ATOM	3136	OH2	WAT	S	149	37.145	57.288	47.392	1.00	36.13	8
ATOM	3137	OH2	WAT	S	150	25.171	18.011	32.273	1.00	38.04	8
ATOM	3138	OH2	WAT	S	151	24.054	43.182	55.583	1.00	41.68	8
ATOM	3139	OH2	WAT	S	152	27.686	64.936	52.937	1.00	60.62	8
ATOM	3140	OH2	WAT	S	153	24.084	39.543	76.589	1.00	22.62	8
ATOM	3141	OH2	WAT	S	154	42.110	10.159	68.662	1.00	46.98	8
ATOM	3142	OH2	WAT	S	155	9.675	22.905	75.335	1.00	26.45	8
ATOM	3143	OH2	WAT	S	156	4.506	34.799	52.857	1.00	33.84	8
ATOM	3144	OH2	WAT	S	157	32.583	35.051	76.446	1.00	36.27	8
ATOM	3145	OH2	WAT	S	158	40.341	58.311	60.390	1.00	54.69	8
ATOM	3146	OH2	WAT	S	159	29.473	58.378	71.881	1.00	28.59	8
ATOM	3147	OH2	WAT	S	160	11.829	60.543	56.138	1.00	37.67	8
ATOM	3148	OH2	WAT	S	161	24.24	48.010	67.935	1.00	56.62	8
ATOM	3149	OH2	WAT	S	162	12.85	33.929	77.503	1.00	29.88	8
ATOM	3150	OH2	WAT	S	163	9.49	26.168	59.687	1.00	15.42	8
ATOM	3151	OH2	WAT	S	164	27.424	16.480	38.895	1.00	36.86	8
ATOM	3152	OH2	WAT	S	165	8.512	56.634	49.614	1.00	30.08	8
ATOM	3153	OH2	WAT	S	166	30.721	13.394	57.919	1.00	39.47	8
ATOM	3154	OH2	WAT	S	167	49.594	38.223	73.903	1.00	29.50	8
ATOM	3155	OH2	WAT	S	168	41.994	48.023	74.119	1.00	38.12	8
ATOM	3156	OH2	WAT	S	169	42.092	39.503	33.116	1.00	24.47	8
ATOM	3157	OH2	WAT	S	170	34.547	12.749	38.054	1.00	38.65	8
ATOM	3158	OH2	WAT	S	171	15.377	60.862	50.791	1.00	32.82	8
ATOM	3159	OH2	WAT	S	172	31.854	42.110	62.950	1.00	42.43	8
ATOM	3160	OH2	WAT	S	173	48.743	44.073	57.626	1.00	34.04	8
ATOM	3161	OH2	WAT	S	174	8.723	50.038	42.232	1.00	32.87	8
ATOM	3162	OH2	WAT	S	175	14.257	18.280	53.455	1.00	40.51	8
ATOM	3163	OH2	WAT	S	176	31.917	37.509	53.943	1.00	40.43	8
ATOM	3164	OH2	WAT	S	177	23.921	47.029	70.642	1.00	47.97	8
ATOM	3165	OH2	WAT	S	178	27.974	47.778	69.949	1.00	62.12	8
ATOM	3166	OH2	WAT	S	179	7.850	25.093	51.345	1.00	50.13	8
ATOM	3167	OH2	WAT	S	180	22.080	48.840	66.463	1.00	53.81	8
ATOM	3168	OH2	WAT	S	181	34.780	48.220	77.419	1.00	30.86	8

116/263
Figure 17-49

ATOM	3169	OH2	WAT	S	182	43.893	35.526	52.018	1.00	47.14	8
ATOM	3170	OH2	WAT	S	183	29.166	21.424	28.950	1.00	45.08	8
ATOM	3171	OH2	WAT	S	184	51.175	51.545	62.599	1.00	33.88	8
ATOM	3172	OH2	WAT	S	185	18.520	46.208	42.323	1.00	50.85	8
ATOM	3173	OH2	WAT	S	186	44.774	30.219	38.653	1.00	45.36	8
ATOM	3174	OH2	WAT	S	187	30.770	9.460	69.837	1.00	32.44	8
ATOM	3175	OH2	WAT	S	188	22.157	39.535	78.736	1.00	37.01	8
ATOM	3176	OH2	WAT	S	189	11.778	50.526	68.987	1.00	41.34	8
ATOM	3177	OH2	WAT	S	190	31.339	60.910	49.439	1.00	21.88	8
ATOM	3178	OH2	WAT	S	191	31.165	14.244	74.907	1.00	27.47	8
ATOM	3179	OH2	WAT	S	192	39.705	15.398	70.464	1.00	47.05	8
ATOM	3180	OH2	WAT	S	193	3.668	34.304	72.937	1.00	39.82	8
ATOM	3181	OH2	WAT	S	194	25.256	9.360	67.925	1.00	33.21	8
ATOM	3182	OH2	WAT	S	195	47.575	17.667	48.773	1.00	40.79	8
ATOM	3183	OH2	WAT	S	196	32.017	13.045	34.633	1.00	37.00	8
ATOM	3184	OH2	WAT	S	197	35.476	7.006	64.436	1.00	49.59	8
ATOM	3185	OH2	WAT	S	198	12.180	16.270	56.288	1.00	47.22	8
ATOM	3186	OH2	WAT	S	199	37.133	21.226	75.963	1.00	38.59	8
ATOM	3187	OH2	WAT	S	200	40.268	15.712	48.199	1.00	39.24	8
ATOM	3188	OH2	WAT	S	201	25.159	17.768	46.858	1.00	49.88	8
ATOM	3189	OH2	WAT	S	202	24.593	27.104	65.727	1.00	53.46	8
ATOM	3190	OH2	WAT	S	203	36.741	20.267	33.858	1.00	41.90	8
ATOM	3191	OH2	WAT	S	204	10.013	53.930	47.546	1.00	48.06	8
ATOM	3192	OH2	WAT	S	205	22.305	16.731	54.471	1.00	27.07	8
ATOM	3193	OH2	WAT	S	206	47.454	34.778	74.101	1.00	47.44	8
ATOM	3194	OH2	WAT	S	207	35.189	55.767	45.193	1.00	59.49	8
ATOM	3195	OH2	WAT	S	208	37.827	18.151	36.382	1.00	45.31	8
ATOM	3196	OH2	WAT	S	209	6.823	37.405	51.989	1.00	58.23	8
ATOM	3197	OH2	WAT	S	210	32.040	43.551	36.157	1.00	30.78	8
ATOM	3198	OH2	WAT	S	211	17.038	52.360	63.283	1.00	34.08	8
ATOM	3199	OH2	WAT	S	212	30.001	18.471	49.568	1.00	33.92	8
ATOM	3200	OH2	WAT	S	213	23.045	28.615	33.729	1.00	44.22	8
ATOM	3201	OH2	WAT	S	214	26.130	61.496	75.246	1.00	40.49	8
ATOM	3202	OH2	WAT	S	215	33.881	32.473	46.604	1.00	39.35	8
ATOM	3203	OH2	WAT	S	216	23.887	45.987	44.362	1.00	36.50	8
ATOM	3204	OH2	WAT	S	217	6.925	42.281	65.917	1.00	34.22	8
ATOM	3205	OH2	WAT	S	218	32.823	8.977	59.213	1.00	27.03	8
END											

117/263

Figure 18-1

				Residue #	X	Y	Z	B	Segment ID
ATOM	1	CB	ALA	A 2	46.725	14.971	138.208	1.00	56.80
ATOM	2	C	ALA	A 2	47.943	12.813	138.561	1.00	58.93
ATOM	3	O	ALA	A 2	48.857	13.292	137.884	1.00	60.99
ATOM	4	N	ALA	A 2	46.995	14.046	140.488	1.00	56.88
ATOM	5	CA	ALA	A 2	46.801	13.697	139.052	1.00	59.41
ATOM	6	N	LYS	A 3	47.890	11.525	138.903	1.00	53.81
ATOM	7	CA	LYS	A 3	48.937	10.591	138.492	1.00	53.62
ATOM	8	CB	LYS	A 3	48.736	9.229	139.156	1.00	50.26
ATOM	9	CG	LYS	A 3	48.917	9.279	140.665	1.00	56.64
ATOM	10	CD	LYS	A 3	48.950	7.891	141.285	1.00	57.18
ATOM	11	CE	LYS	A 3	49.160	7.964	142.796	1.00	56.74
ATOM	12	NZ	LYS	A 3	50.423	8.663	143.165	1.00	54.86
ATOM	13	C	LYS	A 3	49.063	10.430	136.986	1.00	49.95
ATOM	14	O	LYS	A 3	48.088	10.562	136.248	1.00	44.34
ATOM	15	N	VAL	A 4	50.287	10.147	136.550	1.00	46.01
ATOM	16	CA	VAL	A 4	50.609	9.985	135.142	1.00	42.48
ATOM	17	CB	VAL	A 4	51.901	10.755	134.809	1.00	43.42
ATOM	18	CG1	VAL	A 4	52.179	10.713	133.307	1.00	39.20
ATOM	19	CG2	VAL	A 4	51.773	12.186	135.310	1.00	39.34
ATOM	20	C	VAL	A 4	50.787	8.510	134.806	1.00	38.41
ATOM	21	O	VAL	A 4	51.659	7.839	135.351	1.00	37.08
ATOM	22	N	LYS	A 5	49.959	8.011	133.899	1.00	37.79
ATOM	23	CA	LYS	A 5	50.016	6.610	133.515	1.00	38.17
ATOM	24	CB	LYS	A 5	48.700	5.915	133.887	1.00	38.40
ATOM	25	CG	LYS	A 5	48.411	5.803	135.385	1.00	42.84
ATOM	26	CD	LYS	A 5	49.384	4.855	136.070	1.00	44.10
ATOM	27	CE	LYS	A 5	49.017	4.632	137.534	1.00	45.97
ATOM	28	NZ	LYS	A 5	49.045	5.894	138.322	1.00	51.78
ATOM	29	C	LYS	A 5	50.275	6.392	132.030	1.00	38.31
ATOM	30	O	LYS	A 5	49.992	7.253	131.201	1.00	38.13
ATOM	31	N	LEU	A 6	50.817	5.220	131.717	1.00	35.05
ATOM	32	CA	LEU	A 6	51.082	4.818	130.346	1.00	31.46
ATOM	33	CB	LEU	A 6	52.582	4.592	130.133	1.00	28.46
ATOM	34	CG	LEU	A 6	53.094	4.256	128.720	1.00	30.91
ATOM	35	CD1	LEU	A 6	52.618	2.884	128.295	1.00	33.05
ATOM	36	CD2	LEU	A 6	52.630	5.312	127.744	1.00	21.96
ATOM	37	C	LEU	A 6	50.307	3.512	130.164	1.00	30.50
ATOM	38	O	LEU	A 6	50.453	2.581	130.955	1.00	32.82
ATOM	39	N	ILE	A 7	49.459	3.456	129.145	1.00	26.94
ATOM	40	CA	ILE	A 7	48.676	2.255	128.893	1.00	28.29
ATOM	41	CB	ILE	A 7	47.218	2.598	128.493	1.00	28.94
ATOM	42	CG2	ILE	A 7	46.499	1.343	128.041	1.00	32.57
ATOM	43	CG1	ILE	A 7	46.447	3.172	129.688	1.00	36.59
ATOM	44	CD1	ILE	A 7	46.979	4.468	130.236	1.00	46.80
ATOM	45	C	ILE	A 7	49.341	1.470	127.770	1.00	31.09
ATOM	46	O	ILE	A 7	49.600	2.009	126.695	1.00	27.65
ATOM	47	N	GLY	A 8	49.638	0.201	128.029	1.00	27.30
ATOM	48	CA	GLY	A 8	50.277	-0.614	127.016	1.00	25.50
ATOM	49	C	GLY	A 8	50.578	-2.024	127.480	1.00	30.66
ATOM	50	O	GLY	A 8	50.224	-2.421	128.592	1.00	30.02
ATOM	51	N	THR	A 9	51.238	-2.777	126.611	1.00	28.94
ATOM	52	CA	THR	A 9	51.614	-4.156	126.877	1.00	33.63
ATOM	53	CB	THR	A 9	50.393	-5.083	126.857	1.00	36.19
ATOM	54	OG1	THR	A 9	50.827	-6.441	126.992	1.00	34.87
ATOM	55	CG2	THR	A 9	49.633	-4.931	125.548	1.00	36.49
ATOM	56	C	THR	A 9	52.567	-4.637	125.794	1.00	34.83
ATOM	57	O	THR	A 9	52.545	-4.133	124.677	1.00	36.91
ATOM	58	N	LEU	A 10	53.407	-5.609	126.129	1.00	39.15
ATOM	59	CA	LEU	A 10	54.345	-6.167	125.164	1.00	40.21
ATOM	60	CB	LEU	A 10	55.402	-7.009	125.881	1.00	42.40
ATOM	61	CG	LEU	A 10	56.482	-6.282	126.687	1.00	42.29
ATOM	62	CD1	LEU	A 10	55.870	-5.293	127.647	1.00	42.92
ATOM	63	CD2	LEU	A 10	57.319	-7.306	127.424	1.00	40.29
ATOM	64	C	LEU	A 10	53.591	-7.039	124.159	1.00	41.70
ATOM	65	O	LEU	A 10	54.055	-7.266	123.044	1.00	37.13
ATOM	66	N	ASP	A 11	52.419	-7.519	124.557	1.00	47.28

Figure 18-2

ATOM	67	CA	ASP	A	11	51.617	-8.369	123.683	1.00	53.30
ATOM	68	CB	ASP	A	11	50.230	-8.608	124.287	1.00	52.35
ATOM	69	CG	ASP	A	11	50.295	-9.331	125.610	1.00	53.33
ATOM	70	OD1	ASP	A	11	51.004	-10.358	125.685	1.00	52.21
ATOM	71	OD2	ASP	A	11	49.630	-8.883	126.567	1.00	58.48
ATOM	72	C	ASP	A	11	51.459	-7.840	122.257	1.00	53.33
ATOM	73	O	ASP	A	11	51.360	-8.626	121.311	1.00	54.31
ATOM	74	N	TYR	A	12	51.424	-6.521	122.092	1.00	51.92
ATOM	75	CA	TYR	A	12	51.275	-5.970	120.749	1.00	51.41
ATOM	76	CB	TYR	A	12	51.328	-4.437	120.755	1.00	49.05
ATOM	77	CG	TYR	A	12	50.164	-3.729	121.421	1.00	45.48
ATOM	78	CD1	TYR	A	12	50.296	-3.157	122.686	1.00	47.08
ATOM	79	CE1	TYR	A	12	49.252	-2.430	123.263	1.00	47.53
ATOM	80	CD2	TYR	A	12	48.952	-3.565	120.749	1.00	43.77
ATOM	81	CE2	TYR	A	12	47.906	-2.847	121.310	1.00	44.16
ATOM	82	CZ	TYR	A	12	48.061	-2.279	122.566	1.00	48.67
ATOM	83	OH	TYR	A	12	47.030	-1.548	123.116	1.00	48.65
ATOM	84	C	TYR	A	12	52.367	-6.503	119.816	1.00	50.01
ATOM	85	O	TYR	A	12	52.197	-6.525	118.596	1.00	45.56
ATOM	86	N	GLY	A	13	53.484	-6.931	120.396	1.00	48.72
ATOM	87	CA	GLY	A	13	54.574	-7.458	119.599	1.00	50.56
ATOM	88	C	GLY	A	13	54.196	-8.727	118.857	1.00	53.32
ATOM	89	O	GLY	A	13	54.931	-9.184	117.982	1.00	52.64
ATOM	90	N	LYS	A	14	53.045	-9.294	119.207	1.00	53.37
ATOM	91	CA	LYS	A	14	52.555	-10.518	118.579	1.00	54.56
ATOM	92	CB	LYS	A	14	52.022	-11.475	119.653	1.00	58.02
ATOM	93	CG	LYS	A	14	53.086	-12.062	120.591	1.00	62.81
ATOM	94	CD	LYS	A	14	53.934	-13.154	119.918	1.00	61.61
ATOM	95	CE	LYS	A	14	54.747	-12.638	118.734	1.00	61.77
ATOM	96	NZ	LYS	A	14	55.514	-13.713	118.045	1.00	58.35
ATOM	97	C	LYS	A	14	51.455	-10.231	117.559	1.00	52.03
ATOM	98	O	LYS	A	14	50.911	-11.145	116.942	1.00	51.71
ATOM	99	N	TYR	A	15	51.143	-8.955	117.372	1.00	46.92
ATOM	100	CA	TYR	A	15	50.091	-8.563	116.449	1.00	47.99
ATOM	101	CB	TYR	A	15	48.959	-7.915	117.253	1.00	50.40
ATOM	102	CG	TYR	A	15	48.456	-8.793	118.386	1.00	53.01
ATOM	103	CD1	TYR	A	15	48.166	-8.255	119.637	1.00	52.10
ATOM	104	CE1	TYR	A	15	47.722	-9.053	120.685	1.00	51.72
ATOM	105	CD2	TYR	A	15	48.283	-10.166	118.208	1.00	54.67
ATOM	106	CE2	TYR	A	15	47.838	-10.976	119.250	1.00	55.69
ATOM	107	CZ	TYR	A	15	47.561	-10.412	120.485	1.00	54.18
ATOM	108	OH	TYR	A	15	47.130	-11.208	121.520	1.00	55.42
ATOM	109	C	TYR	A	15	50.592	-7.617	115.353	1.00	46.20
ATOM	110	O	TYR	A	15	49.933	-6.635	115.018	1.00	43.72
ATOM	111	N	ARG	A	16	51.758	-7.924	114.791	1.00	46.29
ATOM	112	CA	ARG	A	16	52.347	-7.109	113.727	1.00	45.66
ATOM	113	CB	ARG	A	16	53.779	-7.545	113.441	1.00	50.56
ATOM	114	CG	ARG	A	16	54.677	-7.698	114.636	1.00	56.90
ATOM	115	CD	ARG	A	16	54.992	-6.388	115.315	1.00	60.72
ATOM	116	NE	ARG	A	16	56.021	-6.602	116.328	1.00	66.70
ATOM	117	CZ	ARG	A	16	57.211	-7.141	116.070	1.00	66.68
ATOM	118	NH1	ARG	A	16	57.520	-7.519	114.834	1.00	65.68
ATOM	119	NH2	ARG	A	16	58.093	-7.314	117.046	1.00	66.33
ATOM	120	C	ARG	A	16	51.573	-7.298	112.429	1.00	44.20
ATOM	121	O	ARG	A	16	50.871	-8.293	112.254	1.00	43.41
ATOM	122	N	TYR	A	17	51.715	-6.346	111.514	1.00	39.23
ATOM	123	CA	TYR	A	17	51.067	-6.453	110.215	1.00	38.71
ATOM	124	CB	TYR	A	17	50.913	-5.072	109.565	1.00	33.83
ATOM	125	CG	TYR	A	17	49.744	-4.255	110.084	1.00	27.35
ATOM	126	CD1	TYR	A	17	49.598	-3.982	111.443	1.00	27.25
ATOM	127	CE1	TYR	A	17	48.540	-3.184	111.909	1.00	27.16
ATOM	128	CD2	TYR	A	17	48.807	-3.720	109.204	1.00	25.78
ATOM	129	CE2	TYR	A	17	47.752	-2.925	109.656	1.00	26.34
ATOM	130	CZ	TYR	A	17	47.626	-2.659	111.009	1.00	27.28
ATOM	131	OH	TYR	A	17	46.602	-1.842	111.450	1.00	22.04
ATOM	132	C	TYR	A	17	51.972	-7.350	109.368	1.00	41.52

119/263

Figure 18-3

ATOM	133	O	TYR	A	17	53.150	-7.525	109.683	1.00	35.63
ATOM	134	N	PRO	A	18	51.440	-7.925	108.278	1.00	46.68
ATOM	135	CD	PRO	A	18	50.076	-7.765	107.755	1.00	47.16
ATOM	136	CA	PRO	A	18	52.205	-8.812	107.392	1.00	48.87
ATOM	137	CB	PRO	A	18	51.213	-9.091	106.262	1.00	48.14
ATOM	138	CG	PRO	A	18	50.343	-7.837	106.274	1.00	55.13
ATOM	139	C	PRO	A	18	53.556	-8.303	106.885	1.00	49.67
ATOM	140	O	PRO	A	18	53.788	-7.101	106.766	1.00	49.33
ATOM	141	N	LYS	A	19	54.432	-9.261	106.592	1.00	53.22
ATOM	142	CA	LYS	A	19	55.800	-9.044	106.114	1.00	57.00
ATOM	143	CB	LYS	A	19	56.223	-10.242	105.252	1.00	62.34
ATOM	144	CG	LYS	A	19	55.069	-10.929	104.537	1.00	67.94
ATOM	145	CD	LYS	A	19	54.239	-9.963	103.714	1.00	70.76
ATOM	146	CE	LYS	A	19	53.004	-10.653	103.162	1.00	73.70
ATOM	147	NZ	LYS	A	19	52.116	-9.701	102.442	1.00	79.01
ATOM	148	C	LYS	A	19	56.229	-7.757	105.405	1.00	55.93
ATOM	149	O	LYS	A	19	57.230	-7.150	105.796	1.00	59.86
ATOM	150	N	ASN	A	20	55.515	-7.338	104.367	1.00	49.62
ATOM	151	CA	ASN	A	20	55.925	-6.130	103.652	1.00	50.02
ATOM	152	CB	ASN	A	20	55.829	-6.359	102.143	1.00	50.62
ATOM	153	CG	ASN	A	20	56.729	-7.487	101.670	1.00	51.26
ATOM	154	OD1	ASN	A	20	57.948	-7.437	101.843	1.00	46.88
ATOM	155	ND2	ASN	A	20	56.130	-8.513	101.074	1.00	50.85
ATOM	156	C	ASN	A	20	55.167	-4.862	104.023	1.00	45.50
ATOM	157	O	ASN	A	20	55.481	-3.778	103.533	1.00	45.35
ATOM	158	N	HIS	A	21	54.182	-4.997	104.899	1.00	37.46
ATOM	159	CA	HIS	A	21	53.374	-3.863	105.321	1.00	32.39
ATOM	160	CB	HIS	A	21	52.198	-4.355	106.162	1.00	29.34
ATOM	161	CG	HIS	A	21	51.118	-3.339	106.348	1.00	30.50
ATOM	162	CD2	HIS	A	21	50.999	-2.314	107.223	1.00	22.88
ATOM	163	ND1	HIS	A	21	49.993	-3.298	105.552	1.00	30.15
ATOM	164	CE1	HIS	A	21	49.226	-2.293	105.933	1.00	30.96
ATOM	165	NE2	HIS	A	21	49.814	-1.680	106.945	1.00	36.41
ATOM	166	C	HIS	A	21	54.194	-2.879	106.155	1.00	29.18
ATOM	167	O	HIS	A	21	55.030	-3.279	106.963	1.00	26.92
ATOM	168	N	PRO	A	22	53.965	-1.572	105.969	1.00	31.12
ATOM	169	CD	PRO	A	22	53.027	-0.912	105.043	1.00	29.46
ATOM	170	CA	PRO	A	22	54.702	-0.567	106.739	1.00	29.27
ATOM	171	CB	PRO	A	22	54.012	0.732	106.326	1.00	26.00
ATOM	172	CG	PRO	A	22	53.670	0.434	104.875	1.00	31.52
ATOM	173	C	PRO	A	22	54.624	-0.822	108.253	1.00	29.96
ATOM	174	O	PRO	A	22	55.575	-0.538	108.981	1.00	27.47
ATOM	175	N	LEU	A	23	53.501	-1.371	108.715	1.00	26.64
ATOM	176	CA	LEU	A	23	53.309	-1.644	110.144	1.00	30.44
ATOM	177	CB	LEU	A	23	51.833	-1.428	110.515	1.00	24.09
ATOM	178	CG	LEU	A	23	51.356	0.029	110.479	1.00	25.30
ATOM	179	CD1	LEU	A	23	49.836	0.103	110.668	1.00	17.72
ATOM	180	CD2	LEU	A	23	52.086	0.816	111.574	1.00	24.15
ATOM	181	C	LEU	A	23	53.775	-3.015	110.662	1.00	31.64
ATOM	182	O	LEU	A	23	53.252	-3.512	111.667	1.00	31.00
ATOM	183	N	LYS	A	24	54.753	-3.636	110.012	1.00	28.25
ATOM	184	CA	LYS	A	24	55.200	-4.929	110.513	1.00	30.90
ATOM	185	CB	LYS	A	24	55.718	-5.810	109.372	1.00	36.59
ATOM	186	CG	LYS	A	24	57.178	-5.650	108.982	1.00	40.77
ATOM	187	CD	LYS	A	24	57.546	-4.259	108.535	1.00	44.61
ATOM	188	CE	LYS	A	24	58.858	-4.303	107.755	1.00	50.44
ATOM	189	NZ	LYS	A	24	59.959	-4.990	108.487	1.00	51.30
ATOM	190	C	LYS	A	24	56.282	-4.736	111.581	1.00	32.57
ATOM	191	O	LYS	A	24	56.695	-5.683	112.245	1.00	29.83
ATOM	192	N	ILE	A	25	56.729	-3.497	111.750	1.00	27.06
ATOM	193	CA	ILE	A	25	57.755	-3.200	112.739	1.00	30.45
ATOM	194	CB	ILE	A	25	58.416	-1.822	112.499	1.00	33.37
ATOM	195	CG2	ILE	A	25	59.056	-1.757	111.120	1.00	33.22
ATOM	196	CG1	ILE	A	25	57.361	-0.722	112.662	1.00	30.45
ATOM	197	CD1	ILE	A	25	57.930	0.689	112.700	1.00	33.12
ATOM	198	C	ILE	A	25	57.156	-3.129	114.141	1.00	32.10

Figure 18-4

ATOM	199	O	ILE	A	25	55.967	-2.851	114.310	1.00	28.15
ATOM	200	N	PBO	A	26	57.979	-3.382	115.168	1.00	31.64
ATOM	201	CD	PRO	A	26	59.395	-3.768	115.139	1.00	31.11
ATOM	202	CA	PRO	A	26	57.507	-3.322	116.556	1.00	31.04
ATOM	203	CB	PRO	A	26	58.709	-3.840	117.347	1.00	32.41
ATOM	204	CG	PRO	A	26	59.454	-4.691	116.324	1.00	39.33
ATOM	205	C	PRO	A	26	57.265	-1.840	116.827	1.00	28.42
ATOM	206	O	PRO	A	26	58.001	-0.994	116.315	1.00	22.23
ATOM	207	N	ARG	A	27	56.251	-1.514	117.614	1.00	24.16
ATOM	208	CA	ARG	A	27	55.977	-0.116	117.899	1.00	28.53
ATOM	209	CB	ARG	A	27	54.787	0.358	117.048	1.00	29.77
ATOM	210	CG	ARG	A	27	55.075	0.191	115.554	1.00	29.64
ATOM	211	CD	ARG	A	27	53.918	0.538	114.620	1.00	26.61
ATOM	212	NE	ARG	A	27	53.622	1.965	114.517	1.00	28.52
ATOM	213	CZ	ARG	A	27	52.649	2.591	115.173	1.00	29.70
ATOM	214	NH1	ARG	A	27	51.857	1.924	115.999	1.00	30.17
ATOM	215	NH2	ARG	A	27	52.451	3.889	114.983	1.00	23.25
ATOM	216	C	ARG	A	27	55.746	0.114	119.387	1.00	30.71
ATOM	217	O	ARG	A	27	56.679	0.490	120.113	1.00	24.60
ATOM	218	N	VAL	A	28	54.529	-0.117	119.863	1.00	23.51
ATOM	219	CA	VAL	A	28	54.282	0.093	121.282	1.00	29.33
ATOM	220	CB	VAL	A	28	52.800	-0.124	121.635	1.00	34.56
ATOM	221	CG1	VAL	A	28	52.599	0.002	123.142	1.00	32.42
ATOM	222	CG2	VAL	A	28	51.947	0.908	120.903	1.00	33.77
ATOM	223	C	VAL	A	28	55.158	-0.816	122.145	1.00	29.75
ATOM	224	O	VAL	A	28	55.673	-0.394	123.182	1.00	32.49
ATOM	225	N	SER	A	29	55.341	-2.059	121.718	1.00	26.09
ATOM	226	CA	SER	A	29	56.162	-2.982	122.483	1.00	31.39
ATOM	227	CB	SER	A	29	56.058	-4.399	121.905	1.00	26.92
ATOM	228	CG	SER	A	29	56.562	-4.464	120.579	1.00	33.85
ATOM	229	C	SER	A	29	57.609	-2.482	122.453	1.00	34.77
ATOM	230	O	SER	A	29	58.378	-2.718	123.391	1.00	29.39
ATOM	231	N	LEU	A	30	57.967	-1.778	121.380	1.00	31.20
ATOM	232	CA	LEU	A	30	59.317	-1.234	121.240	1.00	32.03
ATOM	233	CB	LEU	A	30	59.554	-0.668	119.829	1.00	30.86
ATOM	234	CG	LEU	A	30	61.008	-0.550	119.333	1.00	33.22
ATOM	235	CD1	LEU	A	30	61.066	0.484	118.224	1.00	28.76
ATOM	236	CD2	LEU	A	30	61.948	-0.135	120.441	1.00	35.11
ATOM	237	C	LEU	A	30	59.423	-0.089	122.236	1.00	30.29
ATOM	238	O	LEU	A	30	60.397	0.019	122.984	1.00	27.69
ATOM	239	N	LEU	A	31	58.408	0.769	122.232	1.00	27.38
ATOM	240	CA	LEU	A	31	58.372	1.915	123.126	1.00	24.94
ATOM	241	CB	LEU	A	31	57.008	2.596	123.042	1.00	24.92
ATOM	242	CG	LEU	A	31	56.918	4.069	123.460	1.00	30.49
ATOM	243	CD1	LEU	A	31	55.492	4.390	123.881	1.00	24.71
ATOM	244	CD2	LEU	A	31	57.851	4.355	124.603	1.00	27.32
ATOM	245	C	LEU	A	31	58.610	1.429	124.564	1.00	28.18
ATOM	246	O	LEU	A	31	59.489	1.928	125.263	1.00	33.64
ATOM	247	N	LEU	A	32	57.831	0.445	125.000	1.00	30.17
ATOM	248	CA	LEU	A	32	57.965	-0.084	126.357	1.00	30.59
ATOM	249	CB	LEU	A	32	56.944	-1.206	126.601	1.00	30.55
ATOM	250	CG	LEU	A	32	55.458	-0.879	126.402	1.00	29.50
ATOM	251	CD1	LEU	A	32	54.611	-2.107	126.727	1.00	28.31
ATOM	252	CD2	LEU	A	32	55.058	0.273	127.287	1.00	31.92
ATOM	253	C	LEU	A	32	59.376	-0.597	126.657	1.00	33.56
ATOM	254	O	LEU	A	32	59.961	-0.243	127.682	1.00	36.51
ATOM	255	N	ARG	A	33	59.926	-1.429	125.777	1.00	29.75
ATOM	256	CA	ARG	A	33	61.271	-1.953	125.999	1.00	33.49
ATOM	257	CB	ARG	A	33	61.630	-3.003	124.945	1.00	39.50
ATOM	258	CG	ARG	A	33	60.814	-4.283	125.024	1.00	44.40
ATOM	259	CD	ARG	A	33	61.237	-5.256	123.933	1.00	53.68
ATOM	260	NE	ARG	A	33	60.515	-6.522	124.007	1.00	56.66
ATOM	261	CZ	ARG	A	33	60.611	-7.384	125.014	1.00	58.73
ATOM	262	NH1	ARG	A	33	61.402	-7.121	126.045	1.00	59.32
ATOM	263	NH2	ARG	A	33	59.911	-8.511	124.991	1.00	57.91
ATOM	264	C	ARG	A	33	62.314	-0.845	125.978	1.00	31.45

121/263

Figure 18-5

ATOM	265	O	ARG	A	33	63.288	-0.885	126.722	1.00	26.49
ATOM	266	N	PHE	A	34	62.103	0.146	125.123	1.00	32.42
ATOM	267	CA	PHE	A	34	63.042	1.253	125.000	1.00	33.37
ATOM	268	CB	PHE	A	34	62.617	2.180	123.858	1.00	31.68
ATOM	269	CG	PHE	A	34	63.653	3.202	123.486	1.00	29.05
ATOM	270	CD1	PHE	A	34	64.825	2.819	122.838	1.00	29.21
ATOM	271	CD2	PHE	A	34	63.458	4.546	123.781	1.00	28.25
ATOM	272	CE1	PHE	A	34	65.793	3.763	122.484	1.00	29.35
ATOM	273	CE2	PHE	A	34	64.416	5.501	123.435	1.00	32.67
ATOM	274	CZ	PHE	A	34	65.589	5.108	122.783	1.00	29.08
ATOM	275	C	PHE	A	34	63.083	2.042	126.305	1.00	33.47
ATOM	276	O	PHE	A	34	64.155	2.294	126.852	1.00	27.49
ATOM	277	N	LYS	A	35	61.912	2.432	126.802	1.00	29.34
ATOM	278	CA	LYS	A	35	61.848	3.191	128.042	1.00	31.48
ATOM	279	CB	LYS	A	35	60.406	3.576	128.374	1.00	30.82
ATOM	280	CG	LYS	A	35	59.803	4.552	127.395	1.00	32.98
ATOM	281	CD	LYS	A	35	58.404	4.974	127.790	1.00	40.93
ATOM	282	CE	LYS	A	35	57.410	3.827	127.688	1.00	44.56
ATOM	283	NZ	LYS	A	35	57.754	2.656	128.548	1.00	55.10
ATOM	284	C	LYS	A	35	62.443	2.387	129.183	1.00	34.47
ATOM	285	O	LYS	A	35	63.136	2.933	130.043	1.00	32.01
ATOM	286	N	ASP	A	36	62.180	1.086	129.190	1.00	36.28
ATOM	287	CA	ASP	A	36	62.710	0.233	130.242	1.00	37.93
ATOM	288	CB	ASP	A	36	62.145	-1.178	130.126	1.00	41.27
ATOM	289	CG	ASP	A	36	62.731	-2.117	131.157	1.00	43.77
ATOM	290	OD1	ASP	A	36	62.660	-1.793	132.360	1.00	43.92
ATOM	291	OD2	ASP	A	36	63.261	-3.178	130.765	1.00	45.78
ATOM	292	C	ASP	A	36	64.227	0.181	130.174	1.00	38.74
ATOM	293	O	ASP	A	36	64.902	0.187	131.201	1.00	36.23
ATOM	294	N	ALA	A	37	64.760	0.127	128.958	1.00	37.96
ATOM	295	CA	ALA	A	37	66.201	0.080	128.768	1.00	39.49
ATOM	296	CB	ALA	A	37	66.525	-0.158	127.299	1.00	39.74
ATOM	297	C	ALA	A	37	66.832	1.386	129.244	1.00	40.09
ATOM	298	O	ALA	A	37	67.962	1.402	129.714	1.00	38.80
ATOM	299	N	MET	A	38	66.085	2.477	129.131	1.00	39.04
ATOM	300	CA	MET	A	38	66.567	3.789	129.545	1.00	38.71
ATOM	301	CB	MET	A	38	65.965	4.863	128.640	1.00	36.66
ATOM	302	CG	MET	A	38	66.335	4.744	127.173	1.00	39.16
ATOM	303	SD	MET	A	38	68.005	5.298	126.840	1.00	37.55
ATOM	304	CE	MET	A	38	67.892	7.033	127.287	1.00	35.74
ATOM	305	C	MET	A	38	66.187	4.094	130.995	1.00	40.58
ATOM	306	O	MET	A	38	66.484	5.173	131.502	1.00	38.12
ATOM	307	N	ASN	A	39	65.530	3.147	131.657	1.00	38.41
ATOM	308	CA	ASN	A	39	65.094	3.346	133.039	1.00	42.46
ATOM	309	CB	ASN	A	39	66.298	3.494	133.979	1.00	46.06
ATOM	310	CG	ASN	A	39	67.125	2.224	134.074	1.00	51.69
ATOM	311	OD1	ASN	A	39	66.625	1.175	134.487	1.00	54.33
ATOM	312	ND2	ASN	A	39	68.396	2.313	133.695	1.00	49.13
ATOM	313	C	ASN	A	39	64.222	4.594	133.134	1.00	41.19
ATOM	314	O	ASN	A	39	64.375	5.402	134.050	1.00	42.74
ATOM	315	N	LEU	A	40	63.301	4.746	132.188	1.00	40.22
ATOM	316	CA	LEU	A	40	62.427	5.909	132.170	1.00	39.85
ATOM	317	CB	LEU	A	40	62.524	6.610	130.812	1.00	40.42
ATOM	318	CG	LEU	A	40	63.940	7.074	130.447	1.00	40.40
ATOM	319	CD1	LEU	A	40	63.916	7.753	129.088	1.00	32.75
ATOM	320	CD2	LEU	A	40	64.470	8.031	131.513	1.00	38.89
ATOM	321	C	LEU	A	40	60.967	5.610	132.505	1.00	38.97
ATOM	322	O	LEU	A	40	60.076	6.409	132.213	1.00	32.32
ATOM	323	N	ILE	A	41	60.720	4.461	133.124	1.00	38.57
ATOM	324	CA	ILE	A	41	59.363	4.109	133.520	1.00	42.43
ATOM	325	CB	ILE	A	41	58.536	3.575	132.330	1.00	39.13
ATOM	326	CG2	ILE	A	41	59.137	2.271	131.820	1.00	36.51
ATOM	327	CG1	ILE	A	41	57.082	3.367	132.774	1.00	38.71
ATOM	328	CD1	ILE	A	41	56.147	2.920	131.676	1.00	44.09
ATOM	329	C	ILE	A	41	59.376	3.056	134.619	1.00	42.40
ATOM	330	O	ILE	A	41	60.255	2.195	134.654	1.00	43.05

ATOM	331	N	ASP	A	42	58.414	3.148	135.532	1.00	47.83
ATOM	332	CA	ASP	A	42	58.301	2.183	136.620	1.00	49.23
ATOM	333	CB	ASP	A	42	58.243	2.880	137.984	1.00	46.60
ATOM	334	CG	ASP	A	42	59.493	3.688	138.284	1.00	52.63
ATOM	335	OD1	ASP	A	42	60.614	3.146	138.141	1.00	49.28
ATOM	336	OD2	ASP	A	42	59.355	4.866	138.678	1.00	52.47
ATOM	337	C	ASP	A	42	57.034	1.368	136.405	1.00	51.22
ATOM	338	O	ASP	A	42	56.048	1.866	135.864	1.00	48.07
ATOM	339	N	GLU	A	43	57.072	0.111	136.832	1.00	51.41
ATOM	340	CA	GLU	A	43	55.945	-0.792	136.673	1.00	50.67
ATOM	341	CB	GLU	A	43	56.234	-2.094	137.412	1.00	54.49
ATOM	342	CG	GLU	A	43	55.208	-3.178	137.185	1.00	60.55
ATOM	343	CD	GLU	A	43	55.524	-4.432	137.974	1.00	66.12
ATOM	344	OE1	GLU	A	43	54.761	-5.417	137.861	1.00	70.33
ATOM	345	OE2	GLU	A	43	56.536	-4.427	138.711	1.00	67.39
ATOM	346	C	GLU	A	43	54.645	-0.178	137.178	1.00	50.20
ATOM	347	O	GLU	A	43	53.567	-0.475	136.658	1.00	48.27
ATOM	348	N	LYS	A	44	54.755	0.683	138.186	1.00	49.04
ATOM	349	CA	LYS	A	44	53.601	1.356	138.778	1.00	47.56
ATOM	350	CB	LYS	A	44	54.013	2.004	140.112	1.00	54.73
ATOM	351	CG	LYS	A	44	53.190	3.229	140.542	1.00	58.07
ATOM	352	CD	LYS	A	44	53.705	4.500	139.853	1.00	61.24
ATOM	353	CE	LYS	A	44	52.849	5.727	140.151	1.00	61.93
ATOM	354	NZ	LYS	A	44	51.501	5.644	139.519	1.00	62.80
ATOM	355	C	LYS	A	44	52.929	2.387	137.875	1.00	44.52
ATOM	356	O	LYS	A	44	51.752	2.701	138.052	1.00	45.31
ATOM	357	N	GLU	A	45	53.674	2.915	136.914	1.00	41.03
ATOM	358	CA	GLU	A	45	53.140	3.914	135.994	1.00	41.23
ATOM	359	CB	GLU	A	45	54.271	4.810	135.500	1.00	38.52
ATOM	360	CG	GLU	A	45	54.973	5.572	136.589	1.00	40.30
ATOM	361	CD	GLU	A	45	56.241	6.222	136.096	1.00	38.06
ATOM	362	OE1	GLU	A	45	57.170	5.478	135.715	1.00	36.93
ATOM	363	OE2	GLU	A	45	56.306	7.467	136.084	1.00	32.57
ATOM	364	C	GLU	A	45	52.479	3.253	134.791	1.00	40.69
ATOM	365	O	GLU	A	45	51.783	3.907	134.015	1.00	39.77
ATOM	366	N	LEU	A	46	52.700	1.953	134.645	1.00	36.90
ATOM	367	CA	LEU	A	46	52.165	1.207	133.517	1.00	40.46
ATOM	368	CB	LEU	A	46	53.222	0.219	133.034	1.00	35.52
ATOM	369	CG	LEU	A	46	52.873	-0.619	131.811	1.00	43.75
ATOM	370	CD1	LEU	A	46	52.571	0.292	130.630	1.00	42.06
ATOM	371	CD2	LEU	A	46	54.035	-1.544	131.500	1.00	42.90
ATOM	372	C	LEU	A	46	50.852	0.467	133.780	1.00	40.03
ATOM	373	O	LEU	A	46	50.741	-0.306	134.730	1.00	39.37
ATOM	374	N	ILE	A	47	49.861	0.718	132.928	1.00	34.03
ATOM	375	CA	ILE	A	47	48.560	0.068	133.033	1.00	32.12
ATOM	376	CB	ILE	A	47	47.413	1.087	132.937	1.00	32.35
ATOM	377	CG2	ILE	A	47	46.069	0.360	132.833	1.00	30.60
ATOM	378	CG1	ILE	A	47	47.448	2.015	134.156	1.00	36.56
ATOM	379	CD1	ILE	A	47	46.372	3.080	134.162	1.00	35.46
ATOM	380	C	ILE	A	47	48.428	-0.920	131.882	1.00	33.67
ATOM	381	O	ILE	A	47	48.505	-0.532	130.717	1.00	27.64
ATOM	382	N	LYS	A	48	48.231	-2.195	132.205	1.00	32.98
ATOM	383	CA	LYS	A	48	48.102	-3.224	131.176	1.00	30.98
ATOM	384	CB	LYS	A	48	48.038	-4.609	131.821	1.00	39.21
ATOM	385	CG	LYS	A	48	47.956	-5.747	130.819	1.00	46.81
ATOM	386	CD	LYS	A	48	47.989	-7.102	131.509	1.00	50.75
ATOM	387	CE	LYS	A	48	47.967	-8.240	130.492	1.00	54.43
ATOM	388	NZ	LYS	A	48	49.151	-8.199	129.580	1.00	50.43
ATOM	389	C	LYS	A	48	46.869	-3.006	130.310	1.00	29.55
ATOM	390	O	LYS	A	48	45.764	-2.840	130.820	1.00	29.65
ATOM	391	N	SER	A	49	47.071	-2.992	128.996	1.00	30.69
ATOM	392	CA	SER	A	49	45.989	-2.802	128.033	1.00	29.32
ATOM	393	CB	SER	A	49	46.551	-2.805	126.609	1.00	31.53
ATOM	394	OG	SER	A	49	47.571	-1.834	126.443	1.00	30.74
ATOM	395	C	SER	A	49	44.952	-3.916	128.147	1.00	31.31
ATOM	396	O	SER	A	49	45.295	-5.059	128.436	1.00	34.44

Figure 18-7

ATOM	397	N	ARG	A	50	43.688	-3.582	127.922	1.00	32.87
ATOM	398	CA	ARG	A	50	42.632	-4.582	127.960	1.00	31.45
ATOM	399	CB	ARG	A	50	41.636	-4.325	129.101	1.00	28.35
ATOM	400	CG	ARG	A	50	40.729	-3.103	128.915	1.00	32.05
ATOM	401	CD	ARG	A	50	39.653	-3.055	130.008	1.00	30.46
ATOM	402	NE	ARG	A	50	38.821	-1.850	129.964	1.00	25.21
ATOM	403	CZ	ARG	A	50	37.930	-1.569	129.016	1.00	28.32
ATOM	404	NH1	ARG	A	50	37.726	-2.406	128.001	1.00	25.45
ATOM	405	NH2	ARG	A	50	37.238	-0.439	129.087	1.00	24.92
ATOM	406	C	ARG	A	50	41.894	-4.470	126.638	1.00	31.12
ATOM	407	O	ARG	A	50	41.895	-3.406	126.019	1.00	24.62
ATOM	408	N	PRO	A	51	41.264	-5.566	126.181	1.00	32.55
ATOM	409	CD	PRO	A	51	41.164	-6.921	126.751	1.00	32.40
ATOM	410	CA	PRO	A	51	40.534	-5.506	124.917	1.00	30.36
ATOM	411	CB	PRO	A	51	40.138	-6.967	124.683	1.00	33.95
ATOM	412	CG	PRO	A	51	41.173	-7.750	125.499	1.00	32.85
ATOM	413	C	PRO	A	51	39.309	-4.630	125.134	1.00	31.61
ATOM	414	O	PRO	A	51	38.877	-4.431	126.267	1.00	29.84
ATOM	415	N	ALA	A	52	38.755	-4.093	124.058	1.00	29.09
ATOM	416	CA	ALA	A	52	37.556	-3.294	124.183	1.00	29.61
ATOM	417	CB	ALA	A	52	37.365	-2.447	122.956	1.00	28.67
ATOM	418	C	ALA	A	52	36.437	-4.321	124.288	1.00	32.39
ATOM	419	O	ALA	A	52	36.603	-5.453	123.844	1.00	30.40
ATOM	420	N	THR	A	53	35.318	-3.947	124.896	1.00	32.98
ATOM	421	CA	THR	A	53	34.192	-4.868	124.997	1.00	36.61
ATOM	422	CB	THR	A	53	33.253	-4.514	126.166	1.00	34.22
ATOM	423	OG1	THR	A	53	32.734	-3.193	125.970	1.00	29.52
ATOM	424	CG2	THR	A	53	33.998	-4.579	127.493	1.00	36.45
ATOM	425	C	THR	A	53	33.411	-4.700	123.702	1.00	38.94
ATOM	426	O	THR	A	53	33.559	-3.689	123.012	1.00	32.67
ATOM	427	N	LYS	A	54	32.577	-5.679	123.372	1.00	39.19
ATOM	428	CA	LYS	A	54	31.792	-5.595	122.152	1.00	40.71
ATOM	429	CB	LYS	A	54	30.933	-6.851	121.994	1.00	41.68
ATOM	430	CG	LYS	A	54	30.367	-7.034	120.597	1.00	49.42
ATOM	431	CD	LYS	A	54	29.541	-8.310	120.508	1.00	51.82
ATOM	432	CE	LYS	A	54	29.075	-8.588	119.087	1.00	52.94
ATOM	433	NZ	LYS	A	54	30.216	-8.879	118.182	1.00	54.26
ATOM	434	C	LYS	A	54	30.913	-4.347	122.237	1.00	39.46
ATOM	435	O	LYS	A	54	30.719	-3.637	121.249	1.00	37.19
ATOM	436	N	GLU	A	55	30.404	-4.075	123.434	1.00	36.71
ATOM	437	CA	GLU	A	55	29.554	-2.913	123.665	1.00	36.18
ATOM	438	CB	GLU	A	55	29.109	-2.877	125.127	1.00	42.16
ATOM	439	CG	GLU	A	55	28.223	-1.694	125.476	1.00	46.04
ATOM	440	CD	GLU	A	55	27.873	-1.639	126.953	1.00	51.15
ATOM	441	OE1	GLU	A	55	27.092	-0.748	127.343	1.00	56.53
ATOM	442	OE2	GLU	A	55	28.382	-2.482	127.727	1.00	51.67
ATOM	443	C	GLU	A	55	30.278	-1.607	123.327	1.00	35.45
ATOM	444	O	GLU	A	55	29.721	-0.729	122.667	1.00	29.11
ATOM	445	N	GLU	A	56	31.518	-1.476	123.776	1.00	27.82
ATOM	446	CA	GLU	A	56	32.289	-0.269	123.497	1.00	34.70
ATOM	447	CB	GLU	A	56	33.635	-0.329	124.232	1.00	30.71
ATOM	448	CG	GLU	A	56	33.474	-0.484	125.746	1.00	35.09
ATOM	449	CD	GLU	A	56	34.787	-0.675	126.479	1.00	32.29
ATOM	450	OE1	GLU	A	56	35.645	-1.434	125.986	1.00	34.54
ATOM	451	OE2	GLU	A	56	34.951	-0.094	127.569	1.00	33.25
ATOM	452	C	GLU	A	56	32.495	-0.104	121.988	1.00	32.51
ATOM	453	O	GLU	A	56	32.341	0.990	121.444	1.00	29.59
ATOM	454	N	LEU	A	57	32.827	-1.196	121.311	1.00	35.58
ATOM	455	CA	LEU	A	57	33.039	-1.147	119.871	1.00	35.70
ATOM	456	CB	LEU	A	57	33.475	-2.512	119.334	1.00	35.25
ATOM	457	CG	LEU	A	57	34.829	-3.030	119.814	1.00	36.19
ATOM	458	CD1	LEU	A	57	35.095	-4.390	119.183	1.00	33.69
ATOM	459	CD2	LEU	A	57	35.925	-2.041	119.433	1.00	32.61
ATOM	460	C	LEU	A	57	31.772	-0.717	119.157	1.00	36.02
ATOM	461	O	LEU	A	57	31.828	0.067	118.205	1.00	32.72
ATOM	462	N	LEU	A	58	30.631	-1.228	119.620	1.00	32.35

124/263

Figure 18-8

ATOM	463	CA	LEU	A	58	29.353	-0.898	119.004	1.00	33.21
ATOM	464	CB	LEU	A	58	28.260	-1.844	119.495	1.00	35.17
ATOM	465	CG	LEU	A	58	28.504	-3.296	119.077	1.00	33.71
ATOM	466	CD1	LEU	A	58	27.338	-4.166	119.524	1.00	36.80
ATOM	467	CD2	LEU	A	58	28.665	-3.364	117.570	1.00	36.50
ATOM	468	C	LEU	A	58	28.940	-0.543	119.222	1.00	30.99
ATOM	469	O	LEU	A	58	27.915	0.985	118.700	1.00	35.50
ATOM	470	N	LEU	A	59	29.733	1.279	119.993	1.00	32.55
ATOM	471	CA	LEU	A	59	29.443	2.687	120.217	1.00	30.37
ATOM	472	CB	LEU	A	59	30.387	3.279	121.268	1.00	28.01
ATOM	473	CG	LEU	A	59	30.174	2.828	122.716	1.00	32.19
ATOM	474	CD1	LEU	A	59	31.248	3.427	123.604	1.00	24.85
ATOM	475	CD2	LEU	A	59	28.785	3.263	123.192	1.00	25.65
ATOM	476	C	LEU	A	59	29.632	3.405	118.890	1.00	31.26
ATOM	477	O	LEU	A	59	29.020	4.442	118.652	1.00	31.80
ATOM	478	N	PHE	A	60	30.482	2.850	118.026	1.00	29.79
ATOM	479	CA	PHE	A	60	30.726	3.454	116.716	1.00	30.24
ATOM	480	CB	PHE	A	60	32.131	4.055	116.637	1.00	29.99
ATOM	481	CG	PHE	A	60	32.443	4.691	115.299	1.00	28.88
ATOM	482	CD1	PHE	A	60	31.706	5.780	114.845	1.00	25.58
ATOM	483	CD2	PHE	A	60	33.448	4.178	114.479	1.00	24.00
ATOM	484	CE1	PHE	A	60	31.959	6.351	113.592	1.00	26.12
ATOM	485	CE2	PHE	A	60	33.709	4.740	113.226	1.00	25.98
ATOM	486	CZ	PHE	A	60	32.963	5.828	112.781	1.00	24.53
ATOM	487	C	PHE	A	60	30.536	2.520	115.529	1.00	30.30
ATOM	488	O	PHE	A	60	29.810	2.854	114.602	1.00	32.82
ATOM	489	N	HIS	A	61	31.195	1.363	115.543	1.00	32.85
ATOM	490	CA	HIS	A	61	31.075	0.418	114.431	1.00	34.59
ATOM	491	CB	HIS	A	61	32.296	-0.492	114.361	1.00	32.89
ATOM	492	CG	HIS	A	61	33.576	0.238	114.116	1.00	34.25
ATOM	493	CD2	HIS	A	61	34.225	0.532	112.967	1.00	34.67
ATOM	494	ND1	HIS	A	61	34.328	0.786	115.133	1.00	37.78
ATOM	495	CE1	HIS	A	61	35.390	1.382	114.619	1.00	37.50
ATOM	496	NE2	HIS	A	61	35.350	1.243	113.307	1.00	37.91
ATOM	497	C	HIS	A	61	29.824	-0.449	114.480	1.00	38.44
ATOM	498	O	HIS	A	61	29.213	-0.612	115.538	1.00	35.78
ATOM	499	N	THR	A	62	29.462	-1.015	113.327	1.00	39.73
ATOM	500	CA	THR	A	62	28.278	-1.868	113.218	1.00	38.05
ATOM	501	CB	THR	A	62	27.682	-1.825	111.804	1.00	37.22
ATOM	502	CG1	THR	A	62	28.631	-2.345	110.867	1.00	41.15
ATOM	503	CG2	THR	A	62	27.348	-0.404	111.418	1.00	38.27
ATOM	504	C	THR	A	62	28.598	-3.317	113.551	1.00	39.06
ATOM	505	O	THR	A	62	29.731	-3.768	113.392	1.00	39.32
ATOM	506	N	GLU	A	63	27.582	-4.034	114.017	1.00	40.92
ATOM	507	CA	GLU	A	63	27.696	-5.441	114.393	1.00	40.68
ATOM	508	CB	GLU	A	63	26.303	-6.000	114.704	1.00	43.19
ATOM	509	CG	GLU	A	63	26.269	-7.451	115.171	1.00	46.90
ATOM	510	CD	GLU	A	63	26.472	-7.593	116.665	1.00	53.11
ATOM	511	OE1	GLU	A	63	26.601	-8.739	117.152	1.00	52.78
ATOM	512	OE2	GLU	A	63	26.487	-6.556	117.358	1.00	57.24
ATOM	513	C	GLU	A	63	28.320	-6.263	113.268	1.00	36.19
ATOM	514	O	GLU	A	63	29.272	-7.011	113.481	1.00	29.70
ATOM	515	N	ASP	A	64	27.755	-6.119	112.074	1.00	35.85
ATOM	516	CA	ASP	A	64	28.198	-6.841	110.886	1.00	37.61
ATOM	517	CB	ASP	A	64	27.363	-6.382	109.697	1.00	43.30
ATOM	518	CG	ASP	A	64	27.313	-4.872	109.582	1.00	53.38
ATOM	519	CD1	ASP	A	64	28.290	-4.269	109.089	1.00	52.15
ATOM	520	CD2	ASP	A	64	26.298	-4.285	110.018	1.00	53.97
ATOM	521	C	ASP	A	64	29.673	-6.660	110.594	1.00	35.04
ATOM	522	O	ASP	A	64	30.379	-7.625	110.303	1.00	33.60
ATOM	523	N	TYR	A	65	30.144	-5.423	110.671	1.00	33.88
ATOM	524	CA	TYR	A	65	31.554	-5.153	110.419	1.00	32.91
ATOM	525	CB	TYR	A	65	31.793	-3.637	110.375	1.00	34.80
ATOM	526	CG	TYR	A	65	33.247	-3.253	110.219	1.00	35.19
ATOM	527	CD1	TYR	A	65	34.009	-3.751	109.163	1.00	28.43
ATOM	528	CE1	TYR	A	65	35.352	-3.411	109.024	1.00	32.52

125/263
Figure 18-9

ATOM	529	CD2	TYR	A	65	33.863	-2.398	111.134	1.00	34.08
ATOM	530	CE2	TYR	A	65	35.211	-2.050	111.002	1.00	29.89
ATOM	531	CZ	TYR	A	65	35.949	-2.560	109.948	1.00	35.29
ATOM	532	OH	TYR	A	65	37.286	-2.231	109.825	1.00	29.81
ATOM	533	C	TYR	A	65	32.405	-5.813	111.504	1.00	27.65
ATOM	534	O	TYR	A	65	33.339	-6.557	111.209	1.00	27.65
ATOM	535	N	ILE	A	66	32.070	-5.559	112.765	1.00	27.32
ATOM	536	CA	ILE	A	66	32.822	-6.153	113.858	1.00	25.82
ATOM	537	CB	ILE	A	66	32.227	-5.764	115.217	1.00	32.25
ATOM	538	CG2	ILE	A	66	33.029	-6.403	116.338	1.00	28.85
ATOM	539	CG1	ILE	A	66	32.226	-4.242	115.364	1.00	31.48
ATOM	540	CD1	ILE	A	66	33.607	-3.612	115.282	1.00	38.02
ATOM	541	C	ILE	A	66	32.836	-7.677	113.736	1.00	31.21
ATOM	542	O	ILE	A	66	33.891	-8.305	113.844	1.00	30.25
ATOM	543	N	ASN	A	67	31.672	-8.279	113.507	1.00	33.28
ATOM	544	CA	ASN	A	67	31.627	-9.731	113.372	1.00	35.87
ATOM	545	CB	ASN	A	67	30.190	-10.242	113.177	1.00	33.07
ATOM	546	CG	ASN	A	67	29.338	-10.072	114.421	1.00	37.34
ATOM	547	OD1	ASN	A	67	29.807	-10.296	115.535	1.00	35.20
ATOM	548	ND2	ASN	A	67	28.071	-9.709	114.236	1.00	34.83
ATOM	549	C	ASN	A	67	32.499	-10.198	112.219	1.00	31.00
ATOM	550	O	ASN	A	67	33.132	-11.248	112.306	1.00	37.26
ATOM	551	N	THR	A	68	32.543	-9.426	111.140	1.00	30.91
ATOM	552	CA	THR	A	68	33.368	-9.814	109.997	1.00	31.04
ATOM	553	CB	THR	A	68	33.133	-8.894	108.792	1.00	34.01
ATOM	554	OG1	THR	A	68	31.780	-9.037	108.352	1.00	33.26
ATOM	555	CG2	THR	A	68	34.072	-9.256	107.646	1.00	30.84
ATOM	556	C	THR	A	68	34.844	-9.794	110.378	1.00	33.31
ATOM	557	O	THR	A	68	35.591	-10.708	110.024	1.00	32.52
ATOM	558	N	LEU	A	69	35.267	-8.768	111.117	1.00	30.30
ATOM	559	CA	LEU	A	69	36.669	-8.686	111.534	1.00	28.20
ATOM	560	CB	LEU	A	69	36.938	-7.409	112.351	1.00	28.25
ATOM	561	CG	LEU	A	69	36.859	-6.049	111.647	1.00	30.18
ATOM	562	CD1	LEU	A	69	37.154	-4.929	112.647	1.00	31.08
ATOM	563	CD2	LEU	A	69	37.868	-6.004	110.505	1.00	27.85
ATOM	564	C	LEU	A	69	37.036	-9.902	112.372	1.00	31.65
ATOM	565	O	LEU	A	69	38.084	-10.319	112.165	1.00	23.95
ATOM	566	N	MET	A	70	36.169	-10.243	113.321	1.00	30.78
ATOM	567	CA	MET	A	70	36.411	-11.383	114.193	1.00	34.50
ATOM	568	CB	MET	A	70	35.318	-11.486	115.258	1.00	31.96
ATOM	569	CG	MET	A	70	35.203	-10.259	116.147	1.00	36.26
ATOM	570	SD	MET	A	70	33.948	-10.454	117.431	1.00	37.52
ATOM	571	CE	MET	A	70	34.633	-11.815	118.403	1.00	37.36
ATOM	572	C	MET	A	70	36.484	-12.685	113.401	1.00	33.33
ATOM	573	O	MET	A	70	37.392	-13.488	113.607	1.00	31.47
ATOM	574	N	GLU	A	71	35.534	-12.887	112.494	1.00	35.37
ATOM	575	CA	GLU	A	71	35.516	-14.098	111.681	1.00	36.6
ATOM	576	CB	GLU	A	71	34.245	-14.160	110.834	1.00	37.37
ATOM	577	CG	GLU	A	71	34.206	-15.359	109.897	1.00	46.37
ATOM	578	CD	GLU	A	71	34.257	-16.693	110.633	1.00	46.37
ATOM	579	OE1	GLU	A	71	34.355	-17.733	109.952	1.00	48.94
ATOM	580	OE2	GLU	A	71	34.190	-16.705	111.882	1.00	45.53
ATOM	581	C	GLU	A	71	36.732	-14.169	110.769	1.00	35.96
ATOM	582	O	GLU	A	71	37.342	-15.228	110.617	1.00	32.99
ATOM	583	N	ALA	A	72	37.079	-13.039	110.159	1.00	36.50
ATOM	584	CA	ALA	A	72	38.225	-12.981	109.264	1.00	33.98
ATOM	585	CB	ALA	A	72	38.366	-11.580	108.675	1.00	33.23
ATOM	586	C	ALA	A	72	39.498	-13.362	109.998	1.00	34.60
ATOM	587	O	ALA	A	72	40.337	-14.094	109.466	1.00	31.53
ATOM	588	N	GLU	A	73	39.647	-12.873	111.224	1.00	30.87
ATOM	589	CA	GLU	A	73	40.847	-13.177	111.985	1.00	29.66
ATOM	590	CB	GLU	A	73	41.004	-12.224	113.180	1.00	33.33
ATOM	591	CG	GLU	A	73	42.234	-12.545	114.033	1.00	32.80
ATOM	592	CD	GLU	A	73	42.390	-11.634	115.233	1.00	40.07
ATOM	593	OE1	GLU	A	73	42.601	-10.418	115.044	1.00	41.02
ATOM	594	OE2	GLU	A	73	42.298	-12.138	116.372	1.00	41.21

126/263 Figure 18-10

ATOM	595	C	GLU	A	73	40.906	-14.615	112.485	1.00	31.73
ATOM	596	O	GLU	A	73	41.957	-15.249	112.409	1.00	32.96
ATOM	597	N	ARG	A	74	39.798	-15.145	112.992	1.00	35.85
ATOM	598	CA	ARG	A	74	39.847	-16.511	113.502	1.00	43.24
ATOM	599	CB	ARG	A	74	38.548	-16.892	114.216	1.00	43.63
ATOM	600	CG	ARG	A	74	37.450	-17.349	113.294	1.00	51.20
ATOM	601	CD	ARG	A	74	36.366	-18.087	114.063	1.00	51.13
ATOM	602	NE	ARG	A	74	35.534	-18.871	113.158	1.00	57.40
ATOM	603	CZ	ARG	A	74	35.991	-19.870	112.403	1.00	56.36
ATOM	604	NH1	ARG	A	74	37.273	-20.208	112.446	1.00	51.10
ATOM	605	NH2	ARG	A	74	35.172	-20.517	111.586	1.00	58.75
ATOM	606	C	ARG	A	74	40.125	-17.506	112.372	1.00	43.06
ATOM	607	O	ARG	A	74	40.916	-18.429	112.541	1.00	42.52
ATOM	608	N	SER	A	75	39.485	-17.305	111.222	1.00	43.63
ATOM	609	CA	SER	A	75	39.670	-18.186	110.066	1.00	44.93
ATOM	610	CB	SER	A	75	38.485	-18.089	109.113	1.00	42.05
ATOM	611	OG	SER	A	75	38.420	-16.799	108.532	1.00	38.43
ATOM	612	C	SER	A	75	40.910	-17.797	109.282	1.00	46.44
ATOM	613	O	SER	A	75	41.339	-18.522	108.383	1.00	45.17
ATOM	614	N	GLN	A	76	41.466	-16.638	109.618	1.00	46.18
ATOM	615	CA	GLN	A	76	42.642	-16.116	108.936	1.00	44.73
ATOM	616	CB	GLN	A	76	43.868	-16.973	109.226	1.00	37.36
ATOM	617	CG	GLN	A	76	45.162	-16.208	109.045	1.00	43.96
ATOM	618	CD	GLN	A	76	45.415	-15.214	110.176	1.00	41.86
ATOM	619	OE1	GLN	A	76	44.499	-14.537	110.655	1.00	37.78
ATOM	620	NE2	GLN	A	76	46.669	-15.111	110.591	1.00	45.00
ATOM	621	C	GLN	A	76	42.374	-16.120	107.429	1.00	44.17
ATOM	622	O	GLN	A	76	43.233	-16.495	106.630	1.00	40.49
ATOM	623	N	SER	A	77	41.168	-15.713	107.053	1.00	43.11
ATOM	624	CA	SER	A	77	40.784	-15.667	105.649	1.00	44.66
ATOM	625	CB	SER	A	77	40.182	-17.004	105.220	1.00	44.56
ATOM	626	OG	SER	A	77	38.974	-17.246	105.925	1.00	42.58
ATOM	627	C	SER	A	77	39.747	-14.573	105.448	1.00	44.80
ATOM	628	O	SER	A	77	39.096	-14.142	106.395	1.00	45.11
ATOM	629	N	VAL	A	78	39.590	-14.137	104.207	1.00	46.06
ATOM	630	CA	VAL	A	78	38.632	-13.095	103.888	1.00	47.65
ATOM	631	CB	VAL	A	78	39.107	-12.245	102.701	1.00	49.63
ATOM	632	CG1	VAL	A	78	38.076	-11.167	102.391	1.00	51.25
ATOM	633	CG2	VAL	A	78	40.454	-11.627	103.017	1.00	53.00
ATOM	634	C	VAL	A	78	37.275	-13.682	103.530	1.00	48.07
ATOM	635	O	VAL	A	78	37.111	-14.301	102.480	1.00	42.31
ATOM	636	N	PRO	A	79	36.282	-13.492	104.407	1.00	49.82
ATOM	637	CD	PRO	A	79	36.347	-12.782	105.696	1.00	50.81
ATOM	638	CA	PRO	A	79	34.927	-13.998	104.186	1.00	51.31
ATOM	639	CB	PRO	A	79	34.170	-13.450	105.396	1.00	53.13
ATOM	640	CG	PRO	A	79	35.244	-13.469	106.469	1.00	53.50
ATOM	641	C	PRO	A	79	34.343	-13.517	102.858	1.00	52.42
ATOM	642	O	PRO	A	79	34.670	-12.428	102.382	1.00	55.73
ATOM	643	N	LYS	A	80	33.482	-14.343	102.273	1.00	49.63
ATOM	644	CA	LYS	A	80	32.824	-14.053	101.002	1.00	51.62
ATOM	645	CB	LYS	A	80	31.632	-15.004	100.822	1.00	53.92
ATOM	646	CG	LYS	A	80	30.817	-14.808	99.545	1.00	56.27
ATOM	647	CD	LYS	A	80	29.586	-15.712	99.560	1.00	56.61
ATOM	648	CE	LYS	A	80	28.744	-15.579	98.298	1.00	56.04
ATOM	649	NZ	LYS	A	80	29.471	-16.036	97.081	1.00	58.90
ATOM	650	C	LYS	A	80	32.338	-12.607	100.874	1.00	51.10
ATOM	651	O	LYS	A	80	31.539	-12.140	101.689	1.00	49.22
ATOM	652	N	GLY	A	81	32.821	-11.914	99.842	1.00	51.14
ATOM	653	CA	GLY	A	81	32.418	-10.537	99.592	1.00	47.07
ATOM	654	C	GLY	A	81	32.876	-9.496	100.599	1.00	46.90
ATOM	655	O	GLY	A	81	32.671	-8.301	100.397	1.00	43.90
ATOM	656	N	ALA	A	82	33.504	-9.942	101.681	1.00	44.50
ATOM	657	CA	ALA	A	82	33.973	-9.029	102.715	1.00	44.69
ATOM	658	CB	ALA	A	82	34.497	-9.825	103.903	1.00	44.62
ATOM	659	C	ALA	A	82	35.049	-8.073	102.215	1.00	41.82
ATOM	660	O	ALA	A	82	35.132	-6.925	102.662	1.00	35.92

127/263

Figure 18-11

ATOM	661	N	ARG	A	83	35.874	-8.549	101.289	1.00	43.30
ATOM	662	CA	ARG	A	83	36.959	-7.742	100.741	1.00	43.25
ATOM	663	CB	ARG	A	83	37.715	-8.533	99.677	1.00	46.60
ATOM	664	CG	ARG	A	83	38.988	-7.865	99.222	1.00	51.32
ATOM	665	CD	ARG	A	83	39.636	-8.632	98.086	1.00	55.55
ATOM	666	NE	ARG	A	83	40.995	-8.164	97.810	1.00	64.08
ATOM	667	CZ	ARG	A	83	41.330	-6.905	97.540	1.00	63.01
ATOM	668	NH1	ARG	A	83	40.403	-5.954	97.504	1.00	62.76
ATOM	669	NH2	ARG	A	83	42.599	-6.600	97.304	1.00	59.66
ATOM	670	C	ARG	A	83	36.453	-6.435	100.134	1.00	44.58
ATOM	671	O	ARG	A	83	37.002	-5.365	100.395	1.00	38.05
ATOM	672	N	GLU	A	84	35.404	-6.528	99.323	1.00	41.82
ATOM	673	CA	GLU	A	84	34.824	-5.356	98.678	1.00	41.44
ATOM	674	CB	GLU	A	84	34.145	-5.765	97.367	1.00	46.27
ATOM	675	CG	GLU	A	84	33.621	-7.185	97.388	1.00	52.61
ATOM	676	CD	GLU	A	84	34.749	-8.198	97.308	1.00	54.12
ATOM	677	OE1	GLU	A	84	34.555	-9.344	97.764	1.00	59.66
ATOM	678	OE2	GLU	A	84	35.823	-7.850	96.769	1.00	50.30
ATOM	679	C	GLU	A	84	33.831	-4.595	99.545	1.00	37.36
ATOM	680	O	GLU	A	84	33.692	-3.379	99.416	1.00	34.30
ATOM	681	N	LYS	A	85	33.138	-5.301	100.427	1.00	36.00
ATOM	682	CA	LYS	A	85	32.154	-4.646	101.280	1.00	36.95
ATOM	683	CB	LYS	A	85	31.089	-5.649	101.725	1.00	36.60
ATOM	684	CG	LYS	A	85	29.975	-5.042	102.570	1.00	40.72
ATOM	685	CD	LYS	A	85	28.939	-6.092	102.963	1.00	46.21
ATOM	686	CE	LYS	A	85	27.839	-5.487	103.827	1.00	49.06
ATOM	687	NZ	LYS	A	85	26.859	-6.513	104.287	1.00	52.72
ATOM	688	C	LYS	A	85	32.785	-4.008	102.513	1.00	36.48
ATOM	689	O	LYS	A	85	32.353	-2.949	102.966	1.00	32.97
ATOM	690	N	TYR	A	86	33.819	-4.649	103.041	1.00	33.69
ATOM	691	CA	TYR	A	86	34.468	-4.169	104.250	1.00	35.23
ATOM	692	CB	TYR	A	86	34.410	-5.281	105.300	1.00	33.65
ATOM	693	CG	TYR	A	86	32.990	-5.665	105.680	1.00	35.09
ATOM	694	CD1	TYR	A	86	32.165	-4.765	106.351	1.00	34.06
ATOM	695	CE1	TYR	A	86	30.866	-5.100	106.704	1.00	34.32
ATOM	696	CD2	TYR	A	86	32.470	-6.923	105.365	1.00	33.17
ATOM	697	CE2	TYR	A	86	31.162	-7.271	105.716	1.00	33.91
ATOM	698	CZ	TYR	A	86	30.369	-6.350	106.386	1.00	34.21
ATOM	699	OH	TYR	A	86	29.079	-6.658	106.738	1.00	35.20
ATOM	700	C	TYR	A	86	35.901	-3.672	104.046	1.00	36.09
ATOM	701	O	TYR	A	86	36.552	-3.208	104.984	1.00	36.06
ATOM	702	N	ASN	A	87	36.382	-3.777	102.814	1.00	36.46
ATOM	703	CA	ASN	A	87	37.712	-3.313	102.441	1.00	32.71
ATOM	704	CB	ASN	A	87	37.768	-1.791	102.576	1.00	36.26
ATOM	705	CG	ASN	A	87	38.989	-1.199	101.926	1.00	37.25
ATOM	706	OD1	ASN	A	87	39.305	-1.518	100.784	1.00	36.29
ATOM	707	ND2	ASN	A	87	39.675	-0.320	102.640	1.00	45.25
ATOM	708	C	ASN	A	87	38.855	-3.956	103.217	1.00	34.73
ATOM	709	O	ASN	A	87	39.868	-3.315	103.512	1.00	33.23
ATOM	710	N	ILE	A	88	38.687	-5.237	103.523	1.00	32.48
ATOM	711	CA	ILE	A	88	39.676	-6.018	104.248	1.00	33.65
ATOM	712	CB	ILE	A	88	39.030	-6.732	105.445	1.00	38.66
ATOM	713	CG2	ILE	A	88	40.021	-7.680	106.081	1.00	41.31
ATOM	714	CG1	ILE	A	88	38.536	-5.707	106.461	1.00	40.45
ATOM	715	CD1	ILE	A	88	39.641	-4.953	107.124	1.00	42.25
ATOM	716	C	ILE	A	88	40.251	-7.090	103.318	1.00	37.36
ATOM	717	O	ILE	A	88	39.555	-7.587	102.431	1.00	35.47
ATOM	718	N	GLY	A	89	41.517	-7.446	103.520	1.00	31.52
ATOM	719	CA	GLY	A	89	42.124	-8.477	102.698	1.00	33.53
ATOM	720	C	GLY	A	89	43.134	-7.994	101.675	1.00	34.50
ATOM	721	O	GLY	A	89	43.951	-8.777	101.186	1.00	32.81
ATOM	722	N	GLY	A	90	43.071	-6.710	101.335	1.00	31.39
ATOM	723	CA	GLY	A	90	44.005	-6.158	100.371	1.00	23.90
ATOM	724	C	GLY	A	90	45.340	-5.893	101.040	1.00	28.78
ATOM	725	O	GLY	A	90	45.563	-6.339	102.163	1.00	21.71
ATOM	726	N	TYR	A	91	46.221	-5.155	100.367	1.00	28.26

ATOM	727	CA	TYR	A	91	47.539	-4.850	100.918	1.00	27.34
ATOM	728	CB	TYR	A	91	48.477	-4.365	99.805	1.00	22.62
ATOM	729	CG	TYR	A	91	48.066	-3.039	99.194	1.00	24.28
ATOM	730	CD1	TYR	A	91	48.374	-1.829	99.822	1.00	21.55
ATOM	731	CE1	TYR	A	91	47.970	-0.609	99.275	1.00	24.69
ATOM	732	CE2	TYR	A	91	47.341	-2.997	98.002	1.00	24.86
ATOM	733	CE3	TYR	A	91	46.931	-1.786	97.447	1.00	29.92
ATOM	734	CZ	TYR	A	91	47.250	-0.597	98.086	1.00	29.04
ATOM	735	OH	TYR	A	91	46.861	0.593	97.516	1.00	29.51
ATOM	736	C	TYR	A	91	47.452	-3.777	101.998	1.00	27.52
ATOM	737	O	TYR	A	91	48.314	-3.689	102.869	1.00	27.20
ATOM	738	N	GLU	A	92	46.402	-2.971	101.938	1.00	26.75
ATOM	739	CA	GLU	A	92	46.232	-1.879	102.882	1.00	28.38
ATOM	740	CB	GLU	A	92	45.234	-0.881	102.310	1.00	28.57
ATOM	741	CG	GLU	A	92	45.232	0.471	102.982	1.00	36.94
ATOM	742	CD	GLU	A	92	44.178	1.395	102.396	1.00	37.40
ATOM	743	OE1	GLU	A	92	42.999	1.293	102.794	1.00	31.22
ATOM	744	OE2	GLU	A	92	44.527	2.209	101.516	1.00	40.54
ATOM	745	C	GLU	A	92	45.770	-2.343	104.259	1.00	29.20
ATOM	746	O	GLU	A	92	46.389	-2.015	105.268	1.00	21.86
ATOM	747	N	ASN	A	93	44.687	-3.117	104.286	1.00	26.51
ATOM	748	CA	ASN	A	93	44.109	-3.613	105.527	1.00	24.02
ATOM	749	CB	ASN	A	93	42.727	-2.988	105.690	1.00	24.51
ATOM	750	CG	ASN	A	93	42.738	-1.488	105.405	1.00	28.61
ATOM	751	OD1	ASN	A	93	43.428	-0.727	106.079	1.00	25.30
ATOM	752	ND2	ASN	A	93	41.987	-1.063	104.393	1.00	20.45
ATOM	753	C	ASN	A	93	43.999	-5.132	105.407	1.00	24.79
ATOM	754	O	ASN	A	93	42.905	-5.680	105.291	1.00	21.89
ATOM	755	N	PRO	A	94	45.142	-5.828	105.429	1.00	24.60
ATOM	756	CD	PRO	A	94	46.493	-5.246	105.540	1.00	22.93
ATOM	757	CA	PRO	A	94	45.241	-7.285	105.312	1.00	27.23
ATOM	758	CB	PRO	A	94	46.730	-7.488	105.093	1.00	25.46
ATOM	759	CG	PRO	A	94	47.299	-6.431	106.046	1.00	26.20
ATOM	760	C	PRO	A	94	44.743	-8.112	106.489	1.00	31.04
ATOM	761	O	PRO	A	94	44.411	-7.589	107.558	1.00	29.10
ATOM	762	N	VAL	A	95	44.696	-9.422	106.266	1.00	28.27
ATOM	763	CA	VAL	A	95	44.299	-10.367	107.291	1.00	28.82
ATOM	764	CB	VAL	A	95	43.938	-11.737	106.677	1.00	30.75
ATOM	765	CG1	VAL	A	95	43.745	-12.766	107.776	1.00	33.60
ATOM	766	CG2	VAL	A	95	42.679	-11.611	105.849	1.00	24.87
ATOM	767	C	VAL	A	95	45.503	-10.549	108.204	1.00	29.98
ATOM	768	O	VAL	A	95	46.637	-10.649	107.729	1.00	31.36
ATOM	769	N	SER	A	96	45.264	-10.572	109.510	1.00	29.38
ATOM	770	CA	SER	A	96	46.335	-10.766	110.485	1.00	32.56
ATOM	771	CB	SER	A	96	47.325	-9.600	110.454	1.00	34.15
ATOM	772	CG	SER	A	96	46.758	-8.448	111.051	1.00	28.33
ATOM	773	C	SER	A	96	45.681	-10.804	111.854	1.00	32.10
ATOM	774	O	SER	A	96	44.458	-10.839	111.950	1.00	37.91
ATOM	775	N	TYR	A	97	46.484	-10.795	112.913	1.00	32.57
ATOM	776	CA	TYR	A	97	45.914	-10.801	114.248	1.00	34.95
ATOM	777	CB	TYR	A	97	46.685	-11.735	115.182	1.00	35.47
ATOM	778	CG	TYR	A	97	46.492	-13.187	114.817	1.00	40.65
ATOM	779	CD1	TYR	A	97	47.319	-13.812	113.882	1.00	40.63
ATOM	780	CE1	TYR	A	97	47.083	-15.121	113.475	1.00	42.16
ATOM	781	CD2	TYR	A	97	45.421	-13.910	115.338	1.00	38.82
ATOM	782	CE2	TYR	A	97	45.175	-15.219	114.936	1.00	42.82
ATOM	783	CD	TYR	A	97	46.010	-15.816	114.005	1.00	42.56
ATOM	784	CH	TYR	A	97	45.772	-17.105	113.601	1.00	46.03
ATOM	785	C	TYR	A	97	45.862	-9.394	114.813	1.00	37.56
ATOM	786	O	TYR	A	97	45.501	-9.195	115.998	1.00	39.06
ATOM	787	N	ALA	A	98	46.115	-8.418	113.948	1.00	31.96
ATOM	788	CA	ALA	A	98	46.048	-7.024	114.341	1.00	30.43
ATOM	789	CB	ALA	A	98	47.105	-6.211	113.600	1.00	29.64
ATOM	790	C	ALA	A	98	44.658	-6.533	113.962	1.00	30.35
ATOM	791	O	ALA	A	98	44.099	-5.655	114.612	1.00	31.82
ATOM	792	N	MET	A	99	44.094	-7.130	112.915	1.00	30.40

129/263

Figure 18-13

ATOM	793	CA	MET	A	99	42.788	-6.730	112.420	1.00	27.54
ATOM	794	CB	MET	A	99	42.370	-7.620	111.238	1.00	30.55
ATOM	795	CG	MET	A	99	42.052	-9.071	111.565	1.00	31.59
ATOM	796	SD	MET	A	99	41.902	-10.077	110.053	1.00	30.13
ATOM	797	CE	MET	A	99	40.770	-9.086	109.085	1.00	28.02
ATOM	798	C	MET	A	99	41.703	-6.696	113.490	1.00	28.02
ATOM	799	O	MET	A	99	40.818	-5.842	113.446	1.00	24.53
ATOM	800	N	PHE	A	100	41.752	-7.614	114.449	1.00	26.07
ATOM	801	CA	PHE	A	100	40.759	-7.583	115.516	1.00	30.47
ATOM	802	CB	PHE	A	100	39.738	-8.718	115.404	1.00	30.29
ATOM	803	CG	PHE	A	100	38.693	-8.657	116.475	1.00	29.35
ATOM	804	CD1	PHE	A	100	37.722	-7.662	116.455	1.00	27.01
ATOM	805	CD2	PHE	A	100	38.756	-9.506	117.575	1.00	30.68
ATOM	806	CE1	PHE	A	100	36.834	-7.507	117.519	1.00	31.41
ATOM	807	CE2	PHE	A	100	37.873	-9.356	118.644	1.00	28.39
ATOM	808	CZ	PHE	A	100	36.913	-8.355	118.618	1.00	24.06
ATOM	809	C	PHE	A	100	41.345	-7.616	116.922	1.00	29.67
ATOM	810	O	PHE	A	100	41.028	-6.751	117.740	1.00	29.67
ATOM	811	N	THR	A	101	42.181	-8.610	117.222	1.00	31.30
ATOM	812	CA	THR	A	101	42.770	-8.701	118.562	1.00	31.37
ATOM	813	CB	THR	A	101	43.610	-9.977	118.732	1.00	31.63
ATOM	814	OG1	THR	A	101	42.777	-11.119	118.532	1.00	31.64
ATOM	815	CG2	THR	A	101	44.197	-10.045	120.137	1.00	27.38
ATOM	816	C	THR	A	101	43.647	-7.493	118.884	1.00	31.66
ATOM	817	O	THR	A	101	43.502	-6.875	119.942	1.00	30.71
ATOM	818	N	GLY	A	102	44.562	-7.166	117.976	1.00	27.40
ATOM	819	CA	GLY	A	102	45.430	-6.018	118.193	1.00	27.19
ATOM	820	C	GLY	A	102	44.631	-4.728	118.266	1.00	27.26
ATOM	821	O	GLY	A	102	44.785	-3.940	119.201	1.00	27.68
ATOM	822	N	SER	A	103	43.767	-4.515	117.279	1.00	30.52
ATOM	823	CA	SER	A	103	42.941	-3.314	117.216	1.00	31.91
ATOM	824	CB	SER	A	103	42.085	-3.334	115.949	1.00	34.63
ATOM	825	OG	SER	A	103	42.896	-3.265	114.791	1.00	35.94
ATOM	826	C	SER	A	103	42.046	-3.163	118.441	1.00	32.44
ATOM	827	O	SER	A	103	41.891	-2.065	118.984	1.00	25.78
ATOM	828	N	SER	A	104	41.455	-4.270	118.871	1.00	30.47
ATOM	829	CA	SER	A	104	40.584	-4.251	120.038	1.00	30.22
ATOM	830	CB	SER	A	104	39.978	-5.633	120.265	1.00	23.88
ATOM	831	OG	SER	A	104	39.078	-5.595	121.358	1.00	36.91
ATOM	832	C	SER	A	104	41.367	-3.841	121.282	1.00	28.13
ATOM	833	O	SER	A	104	40.872	-3.098	122.130	1.00	25.16
ATOM	834	N	LEU	A	105	42.594	-4.336	121.386	1.00	29.39
ATOM	835	CA	LEU	A	105	43.445	-4.034	122.530	1.00	29.52
ATOM	836	CB	LEU	A	105	44.684	-4.922	122.471	1.00	32.90
ATOM	837	CG	LEU	A	105	45.461	-5.176	123.754	1.00	40.34
ATOM	838	CD1	LEU	A	105	44.520	-5.723	124.828	1.00	35.95
ATOM	839	CD2	LEU	A	105	46.582	-6.178	123.462	1.00	40.23
ATOM	840	C	LEU	A	105	43.834	-2.552	122.511	1.00	32.09
ATOM	841	O	LEU	A	105	43.896	-1.894	123.554	1.00	30.38
ATOM	842	N	ALA	A	106	44.081	-2.029	121.314	1.00	30.26
ATOM	843	CA	ALA	A	106	44.448	-0.626	121.151	1.00	28.31
ATOM	844	CB	ALA	A	106	44.958	-0.386	119.738	1.00	23.88
ATOM	845	C	ALA	A	106	43.243	0.268	121.434	1.00	26.04
ATOM	846	O	ALA	A	106	43.380	1.376	121.952	1.00	20.63
ATOM	847	N	THR	A	107	42.058	-0.224	121.099	1.00	26.86
ATOM	848	CA	THR	A	107	40.841	0.542	121.322	1.00	25.04
ATOM	849	CB	THR	A	107	39.706	0.007	120.443	1.00	26.50
ATOM	850	OG1	THR	A	107	40.111	0.092	119.069	1.00	24.62
ATOM	851	CG2	THR	A	107	38.439	0.824	120.629	1.00	19.80
ATOM	852	C	THR	A	107	40.450	0.503	122.798	1.00	27.90
ATOM	853	O	THR	A	107	40.039	1.515	123.361	1.00	29.04
ATOM	854	N	GLY	A	108	40.585	-0.662	123.422	1.00	24.01
ATOM	855	CA	GLY	A	108	40.256	-0.767	124.832	1.00	24.86
ATOM	856	C	GLY	A	108	41.181	0.155	125.603	1.00	23.86
ATOM	857	O	GLY	A	108	40.771	0.790	126.572	1.00	26.97
ATOM	858	N	SER	A	109	42.434	0.236	125.158	1.00	23.07

ATOM	859	CA	SER A 109	43.421	1.090	125.807	1.00	20.96
ATOM	860	CB	SER A 109	44.795	0.910	125.160	1.00	24.84
ATOM	861	OG	SER A 109	45.294	-0.393	125.402	1.00	25.84
ATOM	862	C	SER A 109	43.008	2.552	125.759	1.00	21.13
ATOM	863	O	SER A 109	43.323	3.312	126.672	1.00	23.17
ATOM	864	N	THR A 110	42.311	2.949	124.698	1.00	20.83
ATOM	865	CA	THR A 110	41.841	4.327	124.583	1.00	21.84
ATOM	866	CB	THR A 110	41.332	4.648	123.161	1.00	24.33
ATOM	867	OG1	THR A 110	42.452	4.769	122.276	1.00	25.38
ATOM	868	CG2	THR A 110	40.543	5.954	123.144	1.00	21.18
ATOM	869	C	THR A 110	40.725	4.561	125.600	1.00	28.52
ATOM	870	O	THR A 110	40.632	5.637	126.197	1.00	28.27
ATOM	871	N	VAL A 111	39.882	3.558	125.809	1.00	26.88
ATOM	872	CA	VAL A 111	38.811	3.706	126.793	1.00	30.04
ATOM	873	CB	VAL A 111	37.820	2.519	126.742	1.00	29.94
ATOM	874	CG1	VAL A 111	36.737	2.693	127.802	1.00	27.07
ATOM	875	CG2	VAL A 111	37.193	2.431	125.355	1.00	25.26
ATOM	876	C	VAL A 111	39.440	3.797	128.187	1.00	28.10
ATOM	877	O	VAL A 111	38.968	4.539	129.039	1.00	26.06
ATOM	878	N	GLN A 112	40.521	3.056	128.415	1.00	23.92
ATOM	879	CA	GLN A 112	41.188	3.097	129.711	1.00	30.27
ATOM	880	CB	GLN A 112	42.268	2.020	129.804	1.00	28.61
ATOM	881	CG	GLN A 112	41.777	0.629	129.481	1.00	28.90
ATOM	882	CD	GLN A 112	42.883	-0.397	129.564	1.00	28.60
ATOM	883	OE1	GLN A 112	43.344	-0.740	130.653	1.00	29.68
ATOM	884	NE2	GLN A 112	43.333	-0.880	128.409	1.00	22.13
ATOM	885	C	GLN A 112	41.834	4.461	129.931	1.00	29.99
ATOM	886	O	GLN A 112	41.791	5.006	131.035	1.00	28.43
ATOM	887	N	ALA A 113	42.453	5.004	128.885	1.00	28.64
ATOM	888	CA	ALA A 113	43.083	6.315	129.001	1.00	26.62
ATOM	889	CB	ALA A 113	43.693	6.732	127.684	1.00	23.49
ATOM	890	C	ALA A 113	42.005	7.307	129.407	1.00	24.63
ATOM	891	O	ALA A 113	42.232	8.183	130.240	1.00	26.38
ATOM	892	N	ILE A 114	40.824	7.163	128.822	1.00	25.26
ATOM	893	CA	ILE A 114	39.728	8.063	129.145	1.00	27.05
ATOM	894	CB	ILE A 114	38.554	7.887	128.156	1.00	26.93
ATOM	895	CG2	ILE A 114	37.387	8.770	128.576	1.00	25.86
ATOM	896	CG1	ILE A 114	39.008	8.259	126.739	1.00	28.38
ATOM	897	CD1	ILE A 114	37.938	8.105	125.669	1.00	28.64
ATOM	898	C	ILE A 114	39.239	7.823	130.578	1.00	31.36
ATOM	899	O	ILE A 114	38.898	8.770	131.291	1.00	24.56
ATOM	900	N	GLU A 115	39.210	6.563	131.005	1.00	31.17
ATOM	901	CA	GLU A 115	38.750	6.257	132.358	1.00	32.12
ATOM	902	CB	GLU A 115	38.729	4.744	132.607	1.00	32.15
ATOM	903	CG	GLU A 115	37.904	3.947	131.598	1.00	32.84
ATOM	904	CD	GLU A 115	37.875	2.459	131.912	1.00	34.12
ATOM	905	OE1	GLU A 115	38.910	1.910	132.345	1.00	30.36
ATOM	906	OE2	GLU A 115	36.826	1.827	131.699	1.00	31.38
ATOM	907	C	GLU A 115	39.675	6.932	133.357	1.00	31.65
ATOM	908	O	GLU A 115	39.224	7.446	134.383	1.00	29.25
ATOM	909	N	GLU A 116	40.970	6.933	133.053	1.00	31.50
ATOM	910	CA	GLU A 116	41.942	7.564	133.934	1.00	32.34
ATOM	911	CB	GLU A 116	43.367	7.285	133.457	1.00	33.29
ATOM	912	CG	GLU A 116	43.805	5.842	133.633	1.00	32.29
ATOM	913	CD	GLU A 116	43.701	5.378	135.079	1.00	36.87
ATOM	914	OE1	GLU A 116	44.329	6.003	135.961	1.00	34.07
ATOM	915	OE2	GLU A 116	42.993	4.385	135.335	1.00	35.00
ATOM	916	C	GLU A 116	41.702	9.067	134.006	1.00	36.69
ATOM	917	O	GLU A 116	41.863	9.678	135.066	1.00	34.39
ATOM	918	N	PHE A 117	41.317	9.661	132.881	1.00	31.19
ATOM	919	CA	PHE A 117	41.038	11.091	132.841	1.00	28.43
ATOM	920	CB	PHE A 117	40.593	11.509	131.444	1.00	30.14
ATOM	921	CG	PHE A 117	40.044	12.908	131.381	1.00	35.78
ATOM	922	CD1	PHE A 117	40.882	14.006	131.501	1.00	33.39
ATOM	923	CD2	PHE A 117	38.675	13.123	131.225	1.00	38.90
ATOM	924	CE1	PHE A 117	40.372	15.299	131.466	1.00	30.65

ATOM	925	CE2	PHE	A	117	38.153	14.412	131.190	1.00	36.50
ATOM	926	CZ	PHE	A	117	39.003	15.501	131.310	1.00	35.41
ATOM	927	C	PHE	A	117	39.908	11.401	133.811	1.00	32.78
ATOM	928	O	PHE	A	117	39.966	12.377	134.566	1.00	29.82
ATOM	929	N	LEU	A	118	38.874	10.568	133.771	1.00	28.61
ATOM	930	CA	LEU	A	118	37.720	10.751	134.632	1.00	32.00
ATOM	931	CB	LEU	A	118	36.621	9.748	134.263	1.00	29.19
ATOM	932	CG	LEU	A	118	36.098	9.830	132.820	1.00	34.47
ATOM	933	CD1	LEU	A	118	34.962	8.836	132.622	1.00	32.69
ATOM	934	CD2	LEU	A	118	35.612	11.240	132.522	1.00	32.24
ATOM	935	C	LEU	A	118	38.123	10.590	136.094	1.00	31.17
ATOM	936	O	LEU	A	118	37.576	11.260	136.964	1.00	28.32
ATOM	937	N	LYS	A	119	39.083	9.707	136.363	1.00	27.23
ATOM	938	CA	LYS	A	119	39.531	9.497	137.733	1.00	30.95
ATOM	939	CB	LYS	A	119	40.203	8.130	137.884	1.00	26.35
ATOM	940	CG	LYS	A	119	39.293	6.954	137.540	1.00	32.44
ATOM	941	CD	LYS	A	119	39.895	5.624	137.986	1.00	33.31
ATOM	942	CE	LYS	A	119	41.280	5.385	137.411	1.00	33.47
ATOM	943	NZ	LYS	A	119	41.874	4.102	137.904	1.00	33.40
ATOM	944	C	LYS	A	119	40.493	10.594	138.173	1.00	32.65
ATOM	945	O	LYS	A	119	41.050	10.548	139.270	1.00	28.83
ATOM	946	N	GLY	A	120	40.689	11.583	137.308	1.00	33.77
ATOM	947	CA	GLY	A	120	41.571	12.677	137.652	1.00	33.84
ATOM	948	C	GLY	A	120	43.035	12.448	137.340	1.00	34.27
ATOM	949	O	GLY	A	120	43.880	13.227	137.776	1.00	36.80
ATOM	950	N	ASN	A	121	43.347	11.384	136.606	1.00	30.77
ATOM	951	CA	ASN	A	121	44.731	11.122	136.244	1.00	31.73
ATOM	952	CB	ASN	A	121	45.089	9.646	136.437	1.00	29.34
ATOM	953	CG	ASN	A	121	44.856	9.170	137.851	1.00	35.83
ATOM	954	OD1	ASN	A	121	45.190	9.861	138.816	1.00	32.74
ATOM	955	ND2	ASN	A	121	44.304	7.970	137.986	1.00	33.20
ATOM	956	C	ASN	A	121	44.954	11.506	134.790	1.00	32.59
ATOM	957	O	ASN	A	121	44.031	11.952	134.110	1.00	34.69
ATOM	958	N	VAL	A	122	46.186	11.334	134.322	1.00	32.74
ATOM	959	CA	VAL	A	122	46.540	11.653	132.946	1.00	33.59
ATOM	960	CB	VAL	A	122	47.571	12.790	132.882	1.00	36.05
ATOM	961	CG1	VAL	A	122	47.884	13.121	131.438	1.00	37.58
ATOM	962	CG2	VAL	A	122	47.029	14.021	133.602	1.00	37.19
ATOM	963	C	VAL	A	122	47.147	10.397	132.352	1.00	34.47
ATOM	964	O	VAL	A	122	48.053	9.801	132.939	1.00	31.28
ATOM	965	N	ALA	A	123	46.646	9.989	131.196	1.00	28.06
ATOM	966	CA	ALA	A	123	47.142	8.784	130.563	1.00	30.73
ATOM	967	CB	ALA	A	123	46.133	7.666	130.727	1.00	32.69
ATOM	968	C	ALA	A	123	47.466	8.969	129.088	1.00	30.55
ATOM	969	O	ALA	A	123	46.909	9.830	128.406	1.00	32.89
ATOM	970	N	PHE	A	124	48.380	8.136	128.613	1.00	27.53
ATOM	971	CA	PHE	A	124	48.807	8.157	127.229	1.00	26.56
ATOM	972	CB	PHE	A	124	50.261	8.660	127.157	1.00	25.32
ATOM	973	CG	PHE	A	124	50.903	8.544	125.793	1.00	27.84
ATOM	974	CD1	PHE	A	124	50.179	8.785	124.629	1.00	24.77
ATOM	975	CD2	PHE	A	124	52.266	8.266	125.686	1.00	21.79
ATOM	976	CE1	PHE	A	124	50.802	8.753	123.385	1.00	29.19
ATOM	977	CE2	PHE	A	124	52.894	8.235	124.449	1.00	27.38
ATOM	978	CZ	PHE	A	124	52.164	8.478	123.296	1.00	20.91
ATOM	979	C	PHE	A	124	48.671	6.749	126.675	1.00	21.13
ATOM	980	O	PHE	A	124	49.181	5.795	127.260	1.00	25.38
ATOM	981	N	ASN	A	125	47.933	6.624	125.580	1.00	18.87
ATOM	982	CA	ASN	A	125	47.750	5.342	124.905	1.00	25.05
ATOM	983	CB	ASN	A	125	46.271	4.982	124.756	1.00	22.99
ATOM	984	CG	ASN	A	125	46.073	3.784	123.856	1.00	24.08
ATOM	985	OD1	ASN	A	125	46.916	2.888	123.822	1.00	20.46
ATOM	986	ND2	ASN	A	125	44.960	3.748	123.138	1.00	16.10
ATOM	987	C	ASN	A	125	48.380	5.410	123.518	1.00	23.43
ATOM	988	O	ASN	A	125	47.718	5.749	122.542	1.00	23.48
ATOM	989	N	PRO	A	126	49.680	5.103	123.423	1.00	24.55
ATOM	990	CD	PRO	A	126	50.589	4.730	124.519	1.00	22.87

Figure 18-16

ATOM	991	CA	PRO	A	126	50.413	5.130	122.160	1.00	22.39
ATOM	992	CB	PEO	A	126	51.829	4.751	122.594	1.00	18.20
ATOM	993	CG	PRO	A	126	51.564	3.849	123.798	1.00	25.43
ATOM	994	C	PRO	A	126	49.867	4.224	121.058	1.00	23.18
ATOM	995	O	PRO	A	126	50.173	4.436	119.893	1.00	20.12
ATOM	996	N	ALA	A	127	49.058	3.232	121.423	1.00	23.27
ATOM	997	CA	ALA	A	127	48.493	2.306	120.444	1.00	23.89
ATOM	998	CB	ALA	A	127	48.176	0.967	121.118	1.00	24.82
ATOM	999	C	ALA	A	127	47.241	2.864	119.778	1.00	24.76
ATOM	1000	O	ALA	A	127	46.806	2.360	118.745	1.00	28.99
ATOM	1001	N	GLY	A	128	46.666	3.906	120.367	1.00	22.12
ATOM	1002	CA	GLY	A	128	45.461	4.494	119.809	1.00	21.43
ATOM	1003	C	GLY	A	128	45.732	5.521	118.725	1.00	23.55
ATOM	1004	O	GLY	A	128	46.875	5.695	118.291	1.00	23.25
ATOM	1005	N	GLY	A	129	44.680	6.199	118.283	1.00	18.03
ATOM	1006	CA	GLY	A	129	44.822	7.205	117.243	1.00	24.99
ATOM	1007	C	GLY	A	129	44.600	6.655	115.847	1.00	25.11
ATOM	1008	O	GLY	A	129	44.963	7.293	114.857	1.00	24.99
ATOM	1009	N	MET	A	130	44.002	5.470	115.765	1.00	20.01
ATOM	1010	CA	MET	A	130	43.729	4.825	114.481	1.00	23.63
ATOM	1011	CB	MET	A	130	43.360	3.361	114.744	1.00	22.77
ATOM	1012	CG	MET	A	130	44.455	2.661	115.563	1.00	26.30
ATOM	1013	SD	MET	A	130	44.198	0.913	115.989	1.00	26.57
ATOM	1014	CE	MET	A	130	42.665	1.030	116.936	1.00	27.59
ATOM	1015	C	MET	A	130	42.580	5.617	113.869	1.00	23.70
ATOM	1016	O	MET	A	130	41.421	5.199	113.901	1.00	26.28
ATOM	1017	N	HIS	A	131	42.926	6.766	113.294	1.00	20.66
ATOM	1018	CA	HIS	A	131	41.933	7.687	112.775	1.00	20.99
ATOM	1019	CB	HIS	A	131	42.474	9.125	112.891	1.00	21.01
ATOM	1020	CG	HIS	A	131	43.699	9.391	112.069	1.00	28.30
ATOM	1021	CD2	HIS	A	131	44.498	8.549	111.373	1.00	19.65
ATOM	1022	ND1	HIS	A	131	44.246	10.649	111.917	1.00	27.76
ATOM	1023	CE1	HIS	A	131	45.328	10.567	111.163	1.00	20.48
ATOM	1024	NE2	HIS	A	131	45.503	9.302	110.820	1.00	24.18
ATOM	1025	C	HIS	A	131	41.280	7.513	111.416	1.00	23.76
ATOM	1026	O	HIS	A	131	40.453	8.341	111.051	1.00	21.95
ATOM	1027	N	HIS	A	132	41.600	6.449	110.682	1.00	25.12
ATOM	1028	CA	HIS	A	132	41.006	6.257	109.354	1.00	23.32
ATOM	1029	CB	HIS	A	132	42.060	5.715	108.388	1.00	17.87
ATOM	1030	CG	HIS	A	132	43.148	6.689	108.072	1.00	24.79
ATOM	1031	CD2	HIS	A	132	44.496	6.574	108.144	1.00	21.72
ATOM	1032	ND1	HIS	A	132	42.896	7.944	107.556	1.00	13.58
ATOM	1033	CE1	HIS	A	132	44.044	8.558	107.323	1.00	15.41
ATOM	1034	NE2	HIS	A	132	45.028	7.748	107.668	1.00	15.27
ATOM	1035	C	HIS	A	132	39.752	5.386	109.208	1.00	23.38
ATOM	1036	O	HIS	A	132	38.947	5.615	108.304	1.00	24.70
ATOM	1037	N	ALA	A	133	39.587	4.388	110.070	1.00	23.34
ATOM	1038	CA	ALA	A	133	38.453	3.471	109.953	1.00	23.77
ATOM	1039	CB	ALA	A	133	38.515	2.417	111.053	1.00	27.49
ATOM	1040	C	ALA	A	133	37.093	4.145	109.966	1.00	23.02
ATOM	1041	O	ALA	A	133	36.878	5.117	110.691	1.00	25.98
ATOM	1042	N	PHE	A	134	36.179	3.633	109.148	1.00	18.90
ATOM	1043	CA	PHE	A	134	34.831	4.173	109.103	1.00	23.73
ATOM	1044	CB	PHE	A	134	34.317	4.296	107.663	1.00	24.29
ATOM	1045	CG	PHE	A	134	35.119	5.225	106.801	1.00	26.67
ATOM	1046	CD1	PHE	A	134	36.025	4.724	105.867	1.00	28.69
ATOM	1047	CD2	PHE	A	134	34.975	6.605	106.921	1.00	32.49
ATOM	1048	CE1	PHE	A	134	36.775	5.582	105.063	1.00	28.65
ATOM	1049	CE2	PHE	A	134	35.724	7.479	106.119	1.00	27.86
ATOM	1050	CZ	PHE	A	134	36.623	6.967	105.188	1.00	23.93
ATOM	1051	C	PHE	A	134	33.894	3.260	109.884	1.00	25.91
ATOM	1052	O	PHE	A	134	34.270	2.172	110.319	1.00	27.20
ATOM	1053	N	LYS	A	135	32.670	3.728	110.062	1.00	29.14
ATOM	1054	CA	LYS	A	135	31.638	2.984	110.765	1.00	35.26
ATOM	1055	CB	LYS	A	135	30.294	3.628	110.429	1.00	35.86
ATOM	1056	CG	LYS	A	135	29.072	2.779	110.667	1.00	46.26

Figure 18-17

ATOM	1057	CD	LYS	A	135	27.834	3.542	110.211	1.00	47.72
ATOM	1058	CE	LYS	A	135	26.610	2.645	110.169	1.00	53.65
ATOM	1059	NZ	LYS	A	135	26.788	1.549	109.167	1.00	53.27
ATOM	1060	C	LYS	A	135	31.617	1.490	110.414	1.00	35.62
ATOM	1061	O	LYS	A	135	31.609	0.635	111.301	1.00	32.58
ATOM	1062	N	SER	A	136	31.629	1.180	109.122	1.00	35.97
ATOM	1063	CA	SER	A	136	31.555	-0.211	108.684	1.00	38.99
ATOM	1064	CB	SER	A	136	30.172	-0.474	108.083	1.00	38.87
ATOM	1065	OG	SER	A	136	29.146	-0.072	108.975	1.00	43.54
ATOM	1066	C	SER	A	136	32.608	-0.616	107.660	1.00	37.84
ATOM	1067	O	SER	A	136	32.350	-1.491	106.828	1.00	36.33
ATOM	1068	N	ARG	A	137	33.788	-0.008	107.705	1.00	33.23
ATOM	1069	CA	ARG	A	137	34.797	-0.368	106.724	1.00	30.89
ATOM	1070	CB	ARG	A	137	34.456	0.291	105.385	1.00	33.88
ATOM	1071	CG	ARG	A	137	35.009	-0.465	104.201	1.00	44.41
ATOM	1072	CD	ARG	A	137	34.809	0.261	102.880	1.00	46.27
ATOM	1073	NE	ARG	A	137	35.091	-0.645	101.768	1.00	48.87
ATOM	1074	CZ	ARG	A	137	35.352	-0.261	100.526	1.00	48.64
ATOM	1075	NH1	ARG	A	137	35.372	1.029	100.220	1.00	51.82
ATOM	1076	NH2	ARG	A	137	35.592	-1.169	99.589	1.00	49.01
ATOM	1077	C	ARG	A	137	36.209	0.021	107.143	1.00	31.84
ATOM	1078	O	ARG	A	137	36.428	1.079	107.742	1.00	30.36
ATOM	1079	N	ALA	A	138	37.166	-0.845	106.828	1.00	30.06
ATOM	1080	CA	ALA	A	138	38.560	-0.588	107.158	1.00	32.24
ATOM	1081	CB	ALA	A	138	39.367	-1.864	107.048	1.00	31.25
ATOM	1082	C	ALA	A	138	39.095	0.449	106.187	1.00	29.49
ATOM	1083	O	ALA	A	138	38.612	0.551	105.063	1.00	26.11
ATOM	1084	N	ASN	A	139	40.099	1.206	106.615	1.00	29.54
ATOM	1085	CA	ASN	A	139	40.673	2.241	105.767	1.00	26.99
ATOM	1086	CB	ASN	A	139	39.685	3.415	105.662	1.00	24.10
ATOM	1087	CG	ASN	A	139	40.209	4.556	104.811	1.00	28.02
ATOM	1088	OD1	ASN	A	139	40.729	4.334	103.727	1.00	26.90
ATOM	1089	ND2	ASN	A	139	40.050	5.789	105.293	1.00	23.55
ATOM	1090	C	ASN	A	139	42.027	2.713	106.285	1.00	30.17
ATOM	1091	O	ASN	A	139	42.245	2.827	107.497	1.00	27.55
ATOM	1092	N	GLY	A	140	42.944	2.959	105.354	1.00	31.82
ATOM	1093	CA	GLY	A	140	44.277	3.428	105.702	1.00	24.90
ATOM	1094	C	GLY	A	140	45.000	2.696	106.816	1.00	27.79
ATOM	1095	O	GLY	A	140	45.560	3.339	107.705	1.00	23.85
ATOM	1096	N	PHE	A	141	45.006	1.365	106.768	1.00	24.35
ATOM	1097	CA	PHE	A	141	45.679	0.538	107.783	1.00	24.53
ATOM	1098	CB	PHE	A	141	47.031	1.146	108.197	1.00	26.40
ATOM	1099	CG	PHE	A	141	47.997	1.366	107.062	1.00	30.31
ATOM	1100	CD1	PHE	A	141	49.145	2.125	107.269	1.00	31.60
ATOM	1101	CD2	PHE	A	141	47.781	0.811	105.802	1.00	29.44
ATOM	1102	CE1	PHE	A	141	50.066	2.331	106.243	1.00	30.44
ATOM	1103	CE2	PHE	A	141	48.694	1.008	104.770	1.00	27.91
ATOM	1104	CZ	PHE	A	141	49.840	1.771	104.991	1.00	29.38
ATOM	1105	C	PHE	A	141	44.846	0.387	109.056	1.00	23.53
ATOM	1106	O	PHE	A	141	45.194	-0.399	109.941	1.00	23.09
ATOM	1107	N	CYS	A	142	43.760	1.143	109.159	1.00	22.86
ATOM	1108	CA	CYS	A	142	42.925	1.099	110.356	1.00	23.87
ATOM	1109	CB	CYS	A	142	42.472	2.516	110.723	1.00	22.51
ATOM	1110	SG	CYS	A	142	43.828	3.683	111.072	1.00	27.62
ATOM	1111	C	CYS	A	142	41.694	0.205	110.233	1.00	24.20
ATOM	1112	O	CYS	A	142	40.932	0.307	109.272	1.00	24.12
ATOM	1113	N	TYR	A	143	41.498	-0.663	111.219	1.00	23.84
ATOM	1114	CA	TYR	A	143	40.335	-1.546	111.236	1.00	26.07
ATOM	1115	CB	TYR	A	143	40.728	-2.958	111.680	1.00	27.89
ATOM	1116	CG	TYR	A	143	41.829	-3.582	110.855	1.00	27.30
ATOM	1117	CD1	TYR	A	143	43.169	-3.329	111.137	1.00	25.76
ATOM	1118	CE1	TYR	A	143	44.185	-3.875	110.346	1.00	25.77
ATOM	1119	CD2	TYR	A	143	41.526	-4.394	109.762	1.00	25.87
ATOM	1120	CE2	TYR	A	143	42.531	-4.941	108.967	1.00	23.10
ATOM	1121	CZ	TYR	A	143	43.854	-4.679	109.262	1.00	22.93
ATOM	1122	OH	TYR	A	143	44.849	-5.217	108.476	1.00	20.64

134/263

Figure 18-18

ATOM	1123	C	TYR	A	143	39.281	-0.991	112.193	1.00	24.56
ATOM	1124	O	TYR	A	143	38.085	-1.030	111.905	1.00	24.88
ATOM	1125	N	ILE	A	144	39.734	-0.471	113.331	1.00	23.77
ATOM	1126	CA	ILE	A	144	38.833	0.102	114.335	1.00	27.11
ATOM	1127	CB	ILE	A	144	38.871	-0.729	115.643	1.00	24.56
ATOM	1128	CG2	ILE	A	144	37.941	-0.120	116.690	1.00	23.47
ATOM	1129	CG1	ILE	A	144	38.430	-2.169	115.346	1.00	28.51
ATOM	1130	CD1	ILE	A	144	38.535	-3.113	116.539	1.00	28.70
ATOM	1131	C	ILE	A	144	39.248	1.550	114.627	1.00	24.15
ATOM	1132	O	ILE	A	144	40.428	1.843	114.800	1.00	24.42
ATOM	1133	N	ASN	A	145	38.277	2.453	114.669	1.00	22.04
ATOM	1134	CA	ASN	A	145	38.555	3.866	114.920	1.00	21.31
ATOM	1135	CB	ASN	A	145	37.559	4.732	114.133	1.00	18.87
ATOM	1136	CG	ASN	A	145	37.956	6.205	114.091	1.00	22.21
ATOM	1137	OD1	ASN	A	145	38.223	6.823	115.124	1.00	22.47
ATOM	1138	ND2	ASN	A	145	37.978	6.776	112.892	1.00	23.78
ATOM	1139	C	ASN	A	145	38.417	4.141	116.418	1.00	22.63
ATOM	1140	O	ASN	A	145	37.338	4.535	116.880	1.00	22.45
ATOM	1141	N	ASN	A	146	39.495	3.941	117.178	1.00	16.63
ATOM	1142	CA	ASN	A	146	39.423	4.160	118.628	1.00	23.57
ATOM	1143	CB	ASN	A	146	40.708	3.678	119.320	1.00	19.80
ATOM	1144	CG	ASN	A	146	41.924	4.508	118.967	1.00	27.81
ATOM	1145	OD1	ASN	A	146	42.299	5.421	119.704	1.00	19.55
ATOM	1146	ND2	ASN	A	146	42.544	4.202	117.827	1.00	19.55
ATOM	1147	C	ASN	A	146	39.079	5.602	119.023	1.00	26.32
ATOM	1148	O	ASN	A	146	38.452	5.827	120.059	1.00	28.34
ATOM	1149	N	PRO	A	147	39.512	6.605	118.231	1.00	29.46
ATOM	1150	CD	PRO	A	147	40.383	6.637	117.042	1.00	27.18
ATOM	1151	CA	PRO	A	147	39.150	7.972	118.618	1.00	24.15
ATOM	1152	CB	PRO	A	147	39.859	8.815	117.558	1.00	25.13
ATOM	1153	CG	PRO	A	147	41.081	7.959	117.235	1.00	30.05
ATOM	1154	C	PRO	A	147	37.618	8.136	118.578	1.00	26.71
ATOM	1155	O	PRO	A	147	37.017	8.760	119.456	1.00	24.93
ATOM	1156	N	ALA	A	148	36.989	7.557	117.562	1.00	21.42
ATOM	1157	CA	ALA	A	148	35.536	7.633	117.416	1.00	21.03
ATOM	1158	CB	ALA	A	148	35.112	7.044	116.072	1.00	19.98
ATOM	1159	C	ALA	A	148	34.838	6.891	118.552	1.00	20.49
ATOM	1160	O	ALA	A	148	33.822	7.344	119.067	1.00	21.44
ATOM	1161	N	VAL	A	149	35.381	5.739	118.928	1.00	19.20
ATOM	1162	CA	VAL	A	149	34.818	4.950	120.016	1.00	24.61
ATOM	1163	CB	VAL	A	149	35.570	3.608	120.181	1.00	25.96
ATOM	1164	CG1	VAL	A	149	35.158	2.918	121.485	1.00	26.58
ATOM	1165	CG2	VAL	A	149	35.262	2.704	118.995	1.00	25.67
ATOM	1166	C	VAL	A	149	34.947	5.752	121.304	1.00	23.56
ATOM	1167	O	VAL	A	149	33.990	5.887	122.064	1.00	22.52
ATOM	1168	N	GLY	A	150	36.143	6.287	121.536	1.00	24.65
ATOM	1169	CA	GLY	A	150	36.390	7.074	122.731	1.00	22.82
ATOM	1170	C	GLY	A	150	35.477	8.281	122.838	1.00	25.46
ATOM	1171	O	GLY	A	150	34.919	8.564	123.904	1.00	23.17
ATOM	1172	N	ILE	A	151	35.327	9.001	121.733	1.00	24.38
ATOM	1173	CA	ILE	A	151	34.481	10.180	121.716	1.00	22.85
ATOM	1174	CB	ILE	A	151	34.610	10.928	120.371	1.00	24.45
ATOM	1175	CG2	ILE	A	151	33.598	12.077	120.306	1.00	24.71
ATOM	1176	CG1	ILE	A	151	26.041	11.462	120.222	1.00	28.02
ATOM	1177	CD1	ILE	A	151	36.354	12.056	118.854	1.00	27.10
ATOM	1178	C	ILE	A	151	33.018	9.806	121.987	1.00	28.19
ATOM	1179	O	ILE	A	151	32.337	10.482	122.763	1.00	26.37
ATOM	1180	N	GLU	A	152	32.532	8.734	121.364	1.00	26.32
ATOM	1181	CA	GLU	A	152	31.149	8.314	121.601	1.00	30.07
ATOM	1182	CB	GLU	A	152	30.758	7.161	120.672	1.00	29.37
ATOM	1183	CG	GLU	A	152	30.609	7.543	119.194	1.00	27.68
ATOM	1184	CD	GLU	A	152	29.455	8.504	118.946	1.00	31.82
ATOM	1185	OE1	GLU	A	152	29.139	8.777	117.773	1.00	33.51
ATOM	1186	OE2	GLU	A	152	28.862	9.009	119.918	1.00	34.73
ATOM	1187	C	GLU	A	152	31.009	7.879	123.055	1.00	28.00
ATOM	1188	O	GLU	A	152	29.980	8.096	123.683	1.00	31.23

135/263

Figure 18-19

ATOM	1189	N	TYR	A	153	32.054	7.253	123.583	1.00	28.72
ATOM	1190	CA	TYR	A	153	32.066	6.805	124.971	1.00	31.35
ATOM	1191	CB	TYR	A	153	33.427	6.204	125.307	1.00	31.56
ATOM	1192	CG	TYR	A	153	33.617	5.839	126.759	1.00	33.17
ATOM	1193	CD1	TYR	A	153	33.111	4.647	127.280	1.00	35.43
ATOM	1194	CE1	TYR	A	153	33.321	4.298	128.619	1.00	33.52
ATOM	1195	CD2	TYR	A	153	34.329	6.677	127.611	1.00	34.29
ATOM	1196	CE2	TYR	A	153	34.544	6.342	128.944	1.00	35.34
ATOM	1197	CZ	TYR	A	153	34.041	5.154	129.444	1.00	37.50
ATOM	1198	OH	TYR	A	153	34.260	4.835	130.767	1.00	30.10
ATOM	1199	C	TYR	A	153	31.828	8.022	125.857	1.00	32.71
ATOM	1200	O	TYR	A	153	31.026	7.988	126.787	1.00	29.14
ATOM	1201	N	LEU	A	154	32.538	9.102	125.552	1.00	29.65
ATOM	1202	CA	LEU	A	154	32.413	10.332	126.310	1.00	32.87
ATOM	1203	CB	LEU	A	154	33.477	11.329	125.847	1.00	31.46
ATOM	1204	CG	LEU	A	154	34.910	11.053	126.324	1.00	29.68
ATOM	1205	CD1	LEU	A	154	35.898	11.953	125.605	1.00	29.29
ATOM	1206	CD2	LEU	A	154	34.989	11.278	127.829	1.00	27.19
ATOM	1207	C	LEU	A	154	31.020	10.952	126.232	1.00	34.63
ATOM	1208	O	LEU	A	154	30.475	11.379	127.250	1.00	32.58
ATOM	1209	N	ARG	A	155	30.443	10.999	125.035	1.00	36.63
ATOM	1210	CA	ARG	A	155	29.107	11.569	124.869	1.00	38.36
ATOM	1211	CB	ARG	A	155	28.661	11.502	123.405	1.00	36.32
ATOM	1212	CG	ARG	A	155	29.581	12.253	122.460	1.00	43.15
ATOM	1213	CD	ARG	A	155	29.100	12.201	121.023	1.00	41.10
ATOM	1214	NE	ARG	A	155	27.936	13.047	120.768	1.00	44.00
ATOM	1215	CZ	ARG	A	155	27.331	13.140	119.583	1.00	54.07
ATOM	1216	NH1	ARG	A	155	27.772	12.441	118.540	1.00	51.61
ATOM	1217	NH2	ARG	A	155	26.291	13.948	119.424	1.00	51.76
ATOM	1218	C	ARG	A	155	28.112	10.821	125.745	1.00	36.25
ATOM	1219	O	ARG	A	155	27.270	11.433	126.397	1.00	39.00
ATOM	1220	N	LYS	A	156	28.213	9.496	125.765	1.00	36.48
ATOM	1221	CA	LYS	A	156	27.315	8.698	126.587	1.00	39.06
ATOM	1222	CB	LYS	A	156	27.460	7.213	126.256	1.00	41.88
ATOM	1223	CG	LYS	A	156	26.672	6.816	125.020	1.00	51.15
ATOM	1224	CD	LYS	A	156	27.169	7.505	123.781	1.00	55.56
ATOM	1225	CE	LYS	A	156	26.117	7.502	122.676	1.00	55.63
ATOM	1226	NZ	LYS	A	156	24.993	8.425	123.013	1.00	49.15
ATOM	1227	C	LYS	A	156	27.527	8.932	128.076	1.00	39.91
ATOM	1228	O	LYS	A	156	26.636	8.658	128.876	1.00	37.01
ATOM	1229	N	LYS	A	157	28.703	9.431	128.448	1.00	37.73
ATOM	1230	CA	LYS	A	157	28.985	9.725	129.847	1.00	36.52
ATOM	1231	CB	LYS	A	157	30.493	9.700	130.122	1.00	35.64
ATOM	1232	CG	LYS	A	157	31.094	8.308	130.174	1.00	35.44
ATOM	1233	CD	LYS	A	157	30.509	7.510	131.335	1.00	31.28
ATOM	1234	CE	LYS	A	157	31.077	6.106	131.388	1.00	31.48
ATOM	1235	NZ	LYS	A	157	30.464	5.310	132.493	1.00	36.39
ATOM	1236	C	LYS	A	157	28.423	11.097	130.197	1.00	38.12
ATOM	1237	O	LYS	A	157	28.531	11.547	131.336	1.00	37.61
ATOM	1238	N	GLY	A	158	27.842	11.768	129.205	1.00	36.27
ATOM	1239	CA	GLY	A	158	27.257	13.074	129.452	1.00	34.31
ATOM	1240	C	GLY	A	158	27.972	14.293	128.894	1.00	36.36
ATOM	1241	O	GLY	A	158	27.438	15.399	128.963	1.00	32.96
ATOM	1242	N	PHE	A	159	29.170	14.117	128.344	1.00	33.89
ATOM	1243	CA	PHE	A	159	29.892	15.260	127.796	1.00	30.29
ATOM	1244	CB	PHE	A	159	31.346	14.892	127.504	1.00	28.62
ATOM	1245	CG	PHE	A	159	32.137	14.555	128.730	1.00	28.80
ATOM	1246	CD1	PHE	A	159	32.043	13.300	129.310	1.00	30.41
ATOM	1247	CD2	PHE	A	159	32.951	15.513	129.327	1.00	29.37
ATOM	1248	CE1	PHE	A	159	32.749	12.996	130.472	1.00	34.42
ATOM	1249	CE2	PHE	A	159	33.661	15.223	130.488	1.00	31.10
ATOM	1250	CZ	PHE	A	159	33.561	13.963	131.062	1.00	32.32
ATOM	1251	C	PHE	A	159	29.224	15.786	126.536	1.00	28.88
ATOM	1252	O	PHE	A	159	28.765	15.003	125.705	1.00	27.71
ATOM	1253	N	LYS	A	160	29.180	17.110	126.402	1.00	30.20
ATOM	1254	CA	LYS	A	160	28.550	17.766	125.254	1.00	33.98

Figure 18-20

ATOM	1255	CB	LYS	A	160	27.390	18.653	125.719	1.00	36.87
ATOM	1256	CG	LYS	A	160	26.273	17.914	126.419	1.00	39.48
ATOM	1257	CD	LYS	A	160	25.105	18.850	126.723	1.00	48.58
ATOM	1258	CE	LYS	A	160	25.500	20.003	127.651	1.00	50.81
ATOM	1259	NZ	LYS	A	160	25.924	19.534	129.008	1.00	49.79
ATOM	1260	C	LYS	A	160	29.484	18.616	124.394	1.00	32.59
ATOM	1261	O	LYS	A	160	29.093	19.085	123.327	1.00	30.98
ATOM	1262	N	ARG	A	161	30.700	18.846	124.867	1.00	31.43
ATOM	1263	CA	ARG	A	161	31.665	19.626	124.108	1.00	29.97
ATOM	1264	CB	ARG	A	161	31.781	21.048	124.673	1.00	34.45
ATOM	1265	CG	ARG	A	161	30.476	21.854	124.610	1.00	37.63
ATOM	1266	CD	ARG	A	161	30.705	23.321	124.966	1.00	39.01
ATOM	1267	NE	ARG	A	161	31.158	23.503	126.341	1.00	43.76
ATOM	1268	CZ	ARG	A	161	30.389	23.337	127.414	1.00	43.33
ATOM	1269	NH1	ARG	A	161	29.117	22.985	127.274	1.00	45.95
ATOM	1270	NH2	ARG	A	161	30.893	23.518	128.627	1.00	43.74
ATOM	1271	C	ARG	A	161	33.009	18.910	124.161	1.00	32.71
ATOM	1272	O	ARG	A	161	33.792	19.090	125.092	1.00	28.53
ATOM	1273	N	ILE	A	162	33.257	18.087	123.149	1.00	32.50
ATOM	1274	CA	ILE	A	162	34.485	17.313	123.049	1.00	28.52
ATOM	1275	CB	ILE	A	162	34.146	15.821	122.820	1.00	31.42
ATOM	1276	CG2	ILE	A	162	35.407	14.976	122.898	1.00	24.95
ATOM	1277	CG1	ILE	A	162	33.147	15.355	123.879	1.00	30.25
ATOM	1278	CD1	ILE	A	162	32.564	13.977	123.635	1.00	34.27
ATOM	1279	C	ILE	A	162	35.353	17.816	121.886	1.00	26.46
ATOM	1280	O	ILE	A	162	34.876	17.973	120.762	1.00	27.88
ATOM	1281	N	LEU	A	163	36.626	18.067	122.168	1.00	23.13
ATOM	1282	CA	LEU	A	163	37.575	18.534	121.156	1.00	25.74
ATOM	1283	CB	LEU	A	163	38.384	19.729	121.681	1.00	26.25
ATOM	1284	CG	LEU	A	163	39.626	20.138	120.862	1.00	24.39
ATOM	1285	CD1	LEU	A	163	39.213	20.591	119.473	1.00	26.25
ATOM	1286	CD2	LEU	A	163	40.361	21.252	121.560	1.00	27.76
ATOM	1287	C	LEU	A	163	38.547	17.416	120.792	1.00	27.09
ATOM	1288	O	LEU	A	163	39.053	16.721	121.674	1.00	25.25
ATOM	1289	N	TYR	A	164	38.808	17.257	119.496	1.00	26.97
ATOM	1290	CA	TYR	A	164	39.747	16.241	119.010	1.00	26.97
ATOM	1291	CB	TYR	A	164	39.021	15.181	118.179	1.00	23.38
ATOM	1292	CG	TYR	A	164	39.944	14.146	117.565	1.00	21.76
ATOM	1293	CD1	TYR	A	164	40.563	13.179	118.353	1.00	22.49
ATOM	1294	CE1	TYR	A	164	41.419	12.224	117.794	1.00	22.90
ATOM	1295	CD2	TYR	A	164	40.202	14.142	116.194	1.00	18.74
ATOM	1296	CE2	TYR	A	164	41.060	13.190	115.616	1.00	23.36
ATOM	1297	CZ	TYR	A	164	41.663	12.235	116.426	1.00	21.50
ATOM	1298	OH	TYR	A	164	42.506	11.296	115.878	1.00	18.41
ATOM	1299	C	TYR	A	164	40.798	16.923	118.138	1.00	21.67
ATOM	1300	O	TYR	A	164	40.473	17.511	117.112	1.00	19.75
ATOM	1301	N	ILE	A	165	42.057	16.843	118.551	1.00	25.61
ATOM	1302	CA	ILE	A	165	43.149	17.462	117.804	1.00	24.43
ATOM	1303	CB	ILE	A	165	43.963	18.396	118.717	1.00	26.41
ATOM	1304	CG2	ILE	A	165	45.127	19.017	117.937	1.00	19.36
ATOM	1305	CG1	ILE	A	165	43.035	19.482	119.274	1.00	23.36
ATOM	1306	CD1	ILE	A	165	43.685	20.402	120.299	1.00	25.05
ATOM	1307	C	ILE	A	165	44.040	16.365	117.234	1.00	26.91
ATOM	1308	O	ILE	A	165	44.538	15.505	117.971	1.00	21.91
ATOM	1309	N	ASP	A	166	44.242	16.408	115.920	1.00	24.20
ATOM	1310	CA	ASP	A	166	45.022	15.386	115.228	1.00	27.11
ATOM	1311	CB	ASP	A	166	44.140	14.765	114.137	1.00	28.56
ATOM	1312	CG	ASP	A	166	44.699	13.461	113.599	1.00	34.59
ATOM	1313	OD1	ASP	A	166	45.831	13.456	113.068	1.00	30.37
ATOM	1314	OD2	ASP	A	166	43.995	12.437	113.717	1.00	23.27
ATOM	1315	C	ASP	A	166	46.319	15.924	114.614	1.00	24.47
ATOM	1316	O	ASP	A	166	46.295	16.613	113.591	1.00	23.19
ATOM	1317	N	LEU	A	167	47.452	15.597	115.227	1.00	23.43
ATOM	1318	CA	LEU	A	167	48.738	16.068	114.722	1.00	24.67
ATOM	1319	CB	LEU	A	167	49.682	16.382	115.887	1.00	21.90
ATOM	1320	CG	LEU	A	167	49.143	17.444	116.858	1.00	26.62

137/263

Figure 18-21

ATOM	1321	CD1	LEU	A	167	50.249	17.845	117.821	1.00	25.88
ATOM	1322	CD2	LEU	A	167	48.658	18.668	116.092	1.00	22.40
ATOM	1323	C	LEU	A	167	49.405	15.092	113.755	1.00	25.82
ATOM	1324	O	LEU	A	167	50.504	15.345	113.262	1.00	21.89
ATOM	1325	N	ASP	A	168	48.736	13.977	113.488	1.00	24.69
ATOM	1326	CA	ASP	A	168	49.244	12.975	112.555	1.00	24.59
ATOM	1327	CB	ASP	A	168	48.209	11.852	112.410	1.00	27.12
ATOM	1328	CG	ASP	A	168	48.722	10.669	111.608	1.00	28.11
ATOM	1329	C	ASP	A	168	49.423	13.686	111.209	1.00	24.17
ATOM	1330	O	ASP	A	168	48.629	14.559	110.865	1.00	17.18
ATOM	1331	OD1	ASP	A	168	49.085	9.644	112.227	1.00	25.40
ATOM	1332	OD2	ASP	A	168	48.777	10.750	110.364	1.00	34.72
ATOM	1333	N	ALA	A	169	50.448	13.312	110.446	1.00	21.29
ATOM	1334	CA	ALA	A	169	50.693	13.927	109.140	1.00	25.00
ATOM	1335	CB	ALA	A	169	52.068	13.498	108.601	1.00	21.17
ATOM	1336	C	ALA	A	169	49.612	13.636	108.093	1.00	26.57
ATOM	1337	O	ALA	A	169	49.641	14.204	107.000	1.00	26.90
ATOM	1338	N	HIS	A	170	48.673	12.746	108.406	1.00	21.63
ATOM	1339	CA	HIS	A	170	47.592	12.445	107.468	1.00	24.79
ATOM	1340	C	HIS	A	170	46.243	12.867	108.045	1.00	20.98
ATOM	1341	O	HIS	A	170	46.044	12.849	109.255	1.00	24.12
ATOM	1342	CB	HIS	A	170	47.550	10.950	107.131	1.00	23.17
ATOM	1343	CG	HIS	A	170	48.830	10.420	106.570	1.00	30.28
ATOM	1344	ND1	HIS	A	170	49.842	9.982	107.385	1.00	31.00
ATOM	1345	CE1	HIS	A	170	50.825	9.634	106.577	1.00	24.33
ATOM	1346	CD2	HIS	A	170	49.224	10.329	105.273	1.00	22.88
ATOM	1347	NE2	HIS	A	170	50.502	9.828	105.285	1.00	21.89
ATOM	1348	N	HIS	A	171	45.317	13.231	107.171	1.00	21.14
ATOM	1349	CA	HIS	A	171	43.993	13.661	107.591	1.00	25.57
ATOM	1350	CB	HIS	A	171	43.234	14.242	106.404	1.00	22.47
ATOM	1351	CG	HIS	A	171	41.857	14.719	106.746	1.00	29.75
ATOM	1352	CD2	HIS	A	171	41.433	15.648	107.634	1.00	25.58
ATOM	1353	ND1	HIS	A	171	40.721	14.201	106.160	1.00	28.90
ATOM	1354	CE1	HIS	A	171	39.656	14.787	106.676	1.00	25.35
ATOM	1355	NE2	HIS	A	171	40.060	15.669	107.573	1.00	32.40
ATOM	1356	C	HIS	A	171	43.169	12.533	108.204	1.00	29.61
ATOM	1357	O	HIS	A	171	43.169	11.411	107.698	1.00	27.62
ATOM	1358	N	CYS	A	172	42.461	12.852	109.286	1.00	26.52
ATOM	1359	CA	CYS	A	172	41.610	11.897	109.987	1.00	24.82
ATOM	1360	CB	CYS	A	172	41.460	12.322	111.456	1.00	29.47
ATOM	1361	SG	CYS	A	172	40.959	14.065	111.717	1.00	25.69
ATOM	1362	C	CYS	A	172	40.237	11.797	109.314	1.00	28.21
ATOM	1363	O	CYS	A	172	39.211	12.131	109.914	1.00	26.78
ATOM	1364	N	ASP	A	173	40.213	11.332	108.066	1.00	22.05
ATOM	1365	CA	ASP	A	173	38.949	11.217	107.350	1.00	27.39
ATOM	1366	CB	ASP	A	173	39.167	10.646	105.931	1.00	30.47
ATOM	1367	CG	ASP	A	173	39.824	9.264	105.922	1.00	29.77
ATOM	1368	OD1	ASP	A	173	39.886	8.658	104.830	1.00	21.14
ATOM	1369	OD2	ASP	A	173	40.288	8.787	106.978	1.00	30.04
ATOM	1370	C	ASP	A	173	37.895	10.400	108.105	1.00	27.86
ATOM	1371	O	ASP	A	173	36.720	10.762	108.120	1.00	23.47
ATOM	1372	N	GLY	A	174	38.309	9.315	108.753	1.00	25.84
ATOM	1373	CA	GLY	A	174	37.344	8.513	109.490	1.00	28.49
ATOM	1374	C	GLY	A	174	36.694	9.296	110.619	1.00	26.14
ATOM	1375	O	GLY	A	174	35.475	9.287	110.780	1.00	21.39
ATOM	1376	N	VAL	A	175	37.510	9.984	111.409	1.00	27.24
ATOM	1377	CA	VAL	A	175	36.995	10.773	112.523	1.00	25.53
ATOM	1378	CB	VAL	A	175	38.137	11.299	113.401	1.00	30.54
ATOM	1379	CG1	VAL	A	175	37.565	12.105	114.566	1.00	28.02
ATOM	1380	CG2	VAL	A	175	38.973	10.129	113.911	1.00	21.30
ATOM	1381	C	VAL	A	175	36.163	11.955	112.035	1.00	25.01
ATOM	1382	O	VAL	A	175	35.130	12.282	112.623	1.00	21.60
ATOM	1383	N	GLN	A	176	36.601	12.594	110.957	1.00	25.43
ATOM	1384	CA	GLN	A	176	35.854	13.730	110.426	1.00	26.12
ATOM	1385	CB	GLN	A	176	36.554	14.336	109.205	1.00	24.71
ATOM	1386	CG	GLN	A	176	35.682	15.349	108.469	1.00	26.68

Figure 18-22

ATOM	1387	CD	GLN	A	176	36.385	16.002	107.306	1.00	29.54
ATOM	1388	OE1	GLN	A	176	37.382	15.704	107.486	1.00	26.93
ATOM	1389	NE2	GLN	A	176	35.872	15.776	106.099	1.00	27.58
ATOM	1390	C	GLN	A	176	34.446	13.316	110.029	1.00	27.63
ATOM	1391	O	GLN	A	176	33.481	14.021	110.319	1.00	25.93
ATOM	1392	N	GLU	A	177	34.330	12.173	109.362	1.00	32.21
ATOM	1393	CA	GLU	A	177	33.027	11.696	108.915	1.00	32.72
ATOM	1394	CB	GLU	A	177	33.181	10.445	108.053	1.00	34.20
ATOM	1395	CG	GLU	A	177	31.905	10.069	107.329	1.00	39.40
ATOM	1396	CD	GLU	A	177	32.060	8.819	106.497	1.00	41.42
ATOM	1397	OE1	GLU	A	177	32.056	7.712	107.075	1.00	45.91
ATOM	1398	OE2	GLU	A	177	32.206	8.947	105.264	1.00	42.35
ATOM	1399	C	GLU	A	177	32.128	11.377	110.099	1.00	30.54
ATOM	1400	O	GLU	A	177	30.945	11.697	110.093	1.00	25.39
ATOM	1401	N	ALA	A	178	32.707	10.750	111.114	1.00	27.03
ATOM	1402	CA	ALA	A	178	31.971	10.365	112.303	1.00	30.67
ATOM	1403	CB	ALA	A	178	32.905	9.658	113.289	1.00	30.49
ATOM	1404	C	ALA	A	178	31.261	11.519	113.003	1.00	33.21
ATOM	1405	O	ALA	A	178	30.145	11.355	113.493	1.00	28.64
ATOM	1406	N	PHE	A	179	31.888	12.688	113.055	1.00	29.27
ATOM	1407	CA	PHE	A	179	31.256	13.801	113.751	1.00	30.49
ATOM	1408	CB	PHE	A	179	32.071	14.128	115.001	1.00	24.44
ATOM	1409	CG	PHE	A	179	32.469	12.909	115.781	1.00	24.43
ATOM	1410	CD1	PHE	A	179	33.749	12.375	115.657	1.00	25.04
ATOM	1411	CD2	PHE	A	179	31.536	12.233	116.563	1.00	23.09
ATOM	1412	CE1	PHE	A	179	34.103	11.184	116.293	1.00	16.56
ATOM	1413	CE2	PHE	A	179	31.881	11.038	117.204	1.00	26.38
ATOM	1414	CZ	PHE	A	179	33.170	10.515	117.067	1.00	20.30
ATOM	1415	C	PHE	A	179	31.079	15.037	112.891	1.00	31.00
ATOM	1416	O	PHE	A	179	31.006	16.152	113.399	1.00	31.32
ATOM	1417	N	TYR	A	180	30.980	14.828	111.584	1.00	31.68
ATOM	1418	CA	TYR	A	180	30.829	15.925	110.646	1.00	32.76
ATOM	1419	CB	TYR	A	180	30.931	15.378	109.213	1.00	35.12
ATOM	1420	CG	TYR	A	180	31.331	16.406	108.172	1.00	36.27
ATOM	1421	CD1	TYR	A	180	30.427	16.846	107.204	1.00	37.31
ATOM	1422	CE1	TYR	A	180	30.801	17.791	106.244	1.00	34.81
ATOM	1423	CD2	TYR	A	180	32.624	16.937	108.154	1.00	36.32
ATOM	1424	CE2	TYR	A	180	33.007	17.879	107.203	1.00	37.83
ATOM	1425	CZ	TYR	A	180	32.088	18.304	106.250	1.00	36.05
ATOM	1426	OH	TYR	A	180	32.446	19.255	105.323	1.00	28.04
ATOM	1427	C	TYR	A	180	29.518	16.696	110.825	1.00	30.94
ATOM	1428	O	TYR	A	180	29.459	17.894	110.560	1.00	30.42
ATOM	1429	N	ASP	A	181	28.473	16.026	111.299	1.00	31.56
ATOM	1430	CA	ASP	A	181	27.180	16.691	111.444	1.00	37.30
ATOM	1431	CB	ASP	A	181	26.086	15.833	110.807	1.00	37.68
ATOM	1432	CG	ASP	A	181	25.645	14.689	111.705	1.00	39.86
ATOM	1433	OD1	ASP	A	181	26.505	13.963	112.233	1.00	43.25
ATOM	1434	OD2	ASP	A	181	24.425	14.504	111.871	1.00	46.56
ATOM	1435	C	ASP	A	181	26.754	17.044	112.866	1.00	36.81
ATOM	1436	O	ASP	A	181	25.571	17.286	113.109	1.00	33.91
ATOM	1437	N	THR	A	182	27.689	17.066	113.810	1.00	40.86
ATOM	1438	CA	THR	A	182	27.327	17.412	115.184	1.00	38.27
ATOM	1439	CB	THR	A	182	27.433	16.201	116.133	1.00	37.99
ATOM	1440	OG1	THR	A	182	27.013	16.595	117.448	1.00	35.64
ATOM	1441	CG2	THR	A	182	28.869	15.684	116.194	1.00	35.61
ATOM	1442	C	THR	A	182	28.177	18.546	115.746	1.00	39.51
ATOM	1443	O	THR	A	182	29.365	18.673	115.433	1.00	40.07
ATOM	1444	N	ASP	A	183	27.557	19.369	116.582	1.00	37.01
ATOM	1445	CA	ASP	A	183	28.250	20.497	117.181	1.00	37.74
ATOM	1446	CB	ASP	A	183	27.313	21.706	117.228	1.00	35.56
ATOM	1447	CG	ASP	A	183	26.136	21.493	118.155	1.00	38.01
ATOM	1448	OD1	ASP	A	183	25.614	20.357	118.210	1.00	34.94
ATOM	1449	OD2	ASP	A	183	25.720	22.470	118.814	1.00	38.17
ATOM	1450	C	ASP	A	183	28.762	20.161	118.578	1.00	35.27
ATOM	1451	O	ASP	A	183	29.337	21.015	119.251	1.00	35.16
ATOM	1452	N	GLN	A	184	28.562	18.917	119.012	1.00	35.10

139/263

Figure 18-23

ATOM	1453	CA	GLN	A	184	29.030	18.505	120.333	1.00	35.16
ATOM	1454	CB	GLN	A	184	28.155	17.382	120.906	1.00	36.94
ATOM	1455	CG	GLN	A	184	26.663	17.718	120.988	1.00	38.34
ATOM	1456	CD	GLN	A	184	25.881	16.725	121.838	1.00	43.68
ATOM	1457	OE1	GLN	A	184	26.027	15.512	121.696	1.00	35.48
ATOM	1458	NE2	GLN	A	184	25.036	17.243	122.723	1.00	51.06
ATOM	1459	C	GLN	A	184	30.479	18.035	120.253	1.00	36.32
ATOM	1460	O	GLN	A	184	31.135	17.825	121.275	1.00	34.24
ATOM	1461	N	VAL	A	185	30.976	17.883	119.028	1.00	34.51
ATOM	1462	CA	VAL	A	185	32.348	17.443	118.804	1.00	33.59
ATOM	1463	CB	VAL	A	185	32.393	15.990	118.259	1.00	35.11
ATOM	1464	CG1	VAL	A	185	33.834	15.567	118.003	1.00	23.80
ATOM	1465	CG2	VAL	A	185	31.731	15.045	119.242	1.00	26.00
ATOM	1466	C	VAL	A	185	33.053	18.354	117.803	1.00	33.11
ATOM	1467	O	VAL	A	185	32.545	18.593	116.714	1.00	27.73
ATOM	1468	N	PHE	A	186	34.215	18.872	118.184	1.00	31.49
ATOM	1469	CA	PHE	A	186	34.985	19.729	117.291	1.00	30.63
ATOM	1470	CB	PHE	A	186	35.420	21.023	117.991	1.00	30.34
ATOM	1471	CG	PHE	A	186	36.008	22.047	117.051	1.00	30.22
ATOM	1472	CD1	PHE	A	186	35.265	23.156	116.656	1.00	32.23
ATOM	1473	CD2	PHE	A	186	37.284	21.879	116.524	1.00	29.37
ATOM	1474	CE1	PHE	A	186	35.785	24.078	115.748	1.00	27.87
ATOM	1475	CE2	PHE	A	186	37.813	22.794	115.615	1.00	28.54
ATOM	1476	CZ	PHE	A	186	37.064	23.892	115.227	1.00	30.80
ATOM	1477	C	PHE	A	186	36.232	18.952	116.879	1.00	33.38
ATOM	1478	O	PHE	A	186	36.952	18.426	117.729	1.00	28.30
ATOM	1479	N	VAL	A	187	36.478	18.877	115.574	1.00	32.00
ATOM	1480	CA	VAL	A	187	37.645	18.171	115.060	1.00	29.70
ATOM	1481	CB	VAL	A	187	37.252	17.095	114.019	1.00	30.03
ATOM	1482	CG1	VAL	A	187	38.510	16.488	113.405	1.00	27.77
ATOM	1483	CG2	VAL	A	187	36.410	16.003	114.672	1.00	25.98
ATOM	1484	C	VAL	A	187	38.604	19.153	114.392	1.00	31.03
ATOM	1485	O	VAL	A	187	38.215	19.895	113.491	1.00	31.88
ATOM	1486	N	LEU	A	188	39.850	19.157	114.857	1.00	24.88
ATOM	1487	CA	LEU	A	188	40.899	20.010	114.304	1.00	26.92
ATOM	1488	CB	LEU	A	188	41.468	20.959	115.361	1.00	27.04
ATOM	1489	CG	LEU	A	188	42.823	21.565	114.963	1.00	25.15
ATOM	1490	CD1	LEU	A	188	42.686	22.315	113.648	1.00	18.53
ATOM	1491	CD2	LEU	A	188	43.330	22.485	116.068	1.00	28.81
ATOM	1492	C	LEU	A	188	42.022	19.113	113.815	1.00	31.22
ATOM	1493	O	LEU	A	188	42.579	18.333	114.587	1.00	25.83
ATOM	1494	N	SER	A	189	42.369	19.230	112.540	1.00	30.53
ATOM	1495	CA	SER	A	189	43.429	18.399	112.007	1.00	30.13
ATOM	1496	CB	SER	A	189	42.821	17.249	111.199	1.00	33.41
ATOM	1497	CG	SER	A	189	43.837	16.474	110.588	1.00	32.98
ATOM	1498	C	SER	A	189	44.448	19.120	111.143	1.00	27.94
ATOM	1499	O	SER	A	189	44.084	19.891	111.253	1.00	22.14
ATOM	1500	N	LEU	A	190	45.728	18.877	111.423	1.00	24.80
ATOM	1501	CA	LEU	A	190	46.805	19.438	110.614	1.00	22.23
ATOM	1502	CB	LEU	A	190	47.955	20.000	111.459	1.00	23.69
ATOM	1503	CG	LEU	A	190	47.733	21.075	112.522	1.00	28.92
ATOM	1504	CD1	LEU	A	190	49.070	21.780	112.740	1.00	23.01
ATOM	1505	CD2	LEU	A	190	46.691	22.093	112.087	1.00	28.11
ATOM	1506	C	LEU	A	190	47.300	18.210	109.872	1.00	22.69
ATOM	1507	O	LEU	A	190	47.416	17.141	110.465	1.00	16.55
ATOM	1508	N	HIS	A	191	47.599	18.353	108.587	1.00	19.22
ATOM	1509	CA	HIS	A	191	48.046	17.210	107.804	1.00	23.28
ATOM	1510	CB	HIS	A	191	46.870	16.242	107.650	1.00	15.58
ATOM	1511	CG	HIS	A	191	45.591	16.915	107.256	1.00	24.16
ATOM	1512	CD2	HIS	A	191	45.034	17.124	106.038	1.00	17.71
ATOM	1513	ND1	HIS	A	191	44.695	17.419	108.176	1.00	23.76
ATOM	1514	CE1	HIS	A	191	43.644	17.913	107.545	1.00	19.78
ATOM	1515	NE2	HIS	A	191	43.823	17.746	106.246	1.00	27.87
ATOM	1516	C	HIS	A	191	48.570	17.620	106.434	1.00	23.65
ATOM	1517	O	HIS	A	191	48.419	18.761	106.017	1.00	23.89
ATOM	1518	N	GLN	A	192	49.209	16.681	105.746	1.00	23.49

140/263 Figure 18-24

ATOM	1519	CA	GLN A 192	49.718	16.950	104.412	1.00	20.55
ATOM	1520	CB	GLN A 192	50.474	15.738	103.864	1.00	23.63
ATOM	1521	CG	GLN A 192	51.528	15.181	104.797	1.00	24.07
ATOM	1522	CD	GLN A 192	52.110	13.876	104.293	1.00	26.90
ATOM	1523	OE1	GLN A 192	52.986	13.860	103.421	1.00	20.21
ATOM	1524	NE2	GLN A 192	51.605	12.765	104.828	1.00	23.52
ATOM	1525	C	GLN A 192	48.478	17.174	103.570	1.00	21.41
ATOM	1526	O	GLN A 192	47.478	16.466	103.726	1.00	20.15
ATOM	1527	N	SER A 193	48.528	18.167	102.692	1.00	24.36
ATOM	1528	CA	SER A 193	47.397	18.448	101.821	1.00	23.98
ATOM	1529	CB	SER A 193	47.750	19.537	100.820	1.00	24.60
ATOM	1530	OG	SER A 193	46.729	19.660	99.861	1.00	25.83
ATOM	1531	C	SER A 193	46.985	17.200	101.045	1.00	23.74
ATOM	1532	O	SER A 193	47.829	16.492	100.506	1.00	19.80
ATOM	1533	N	PRO A 194	45.674	16.936	100.953	1.00	24.85
ATOM	1534	CD	PRO A 194	44.561	17.719	101.507	1.00	25.08
ATOM	1535	CA	PRO A 194	45.151	15.772	100.235	1.00	29.25
ATOM	1536	CB	PRO A 194	43.641	15.901	100.444	1.00	30.51
ATOM	1537	CG	PRO A 194	43.554	16.643	101.758	1.00	30.21
ATOM	1538	C	PRO A 194	45.527	15.825	98.756	1.00	30.75
ATOM	1539	O	PRO A 194	45.420	14.830	98.041	1.00	30.04
ATOM	1540	N	GLU A 195	45.967	16.991	98.298	1.00	26.28
ATOM	1541	CA	GLU A 195	46.343	17.127	96.898	1.00	31.11
ATOM	1542	CB	GLU A 195	46.738	18.570	96.571	1.00	29.52
ATOM	1543	CG	GLU A 195	45.680	19.600	96.933	1.00	38.32
ATOM	1544	CD	GLU A 195	45.976	20.972	96.352	1.00	44.15
ATOM	1545	OE1	GLU A 195	47.139	21.425	96.434	1.00	44.23
ATOM	1546	OE2	GLU A 195	45.037	21.605	95.825	1.00	45.06
ATOM	1547	C	GLU A 195	47.499	16.193	96.552	1.00	30.81
ATOM	1548	O	GLU A 195	47.582	15.705	95.426	1.00	37.17
ATOM	1549	N	TYR A 196	48.377	15.922	97.515	1.00	25.01
ATOM	1550	CA	TYR A 196	49.517	15.053	97.242	1.00	23.43
ATOM	1551	CB	TYR A 196	50.810	15.881	97.223	1.00	26.67
ATOM	1552	CG	TYR A 196	51.255	16.424	98.572	1.00	26.78
ATOM	1553	CD1	TYR A 196	51.957	15.625	99.476	1.00	26.08
ATOM	1554	CE1	TYR A 196	52.338	16.110	100.734	1.00	26.77
ATOM	1555	CD2	TYR A 196	50.944	17.731	98.958	1.00	27.55
ATOM	1556	CE2	TYR A 196	51.320	18.226	100.216	1.00	25.95
ATOM	1557	CZ	TYR A 196	52.012	17.409	101.096	1.00	24.78
ATOM	1558	OH	TYR A 196	52.356	17.879	102.345	1.00	25.50
ATOM	1559	C	TYR A 196	49.670	13.906	98.229	1.00	27.05
ATOM	1560	O	TYR A 196	50.585	13.088	98.096	1.00	24.02
ATOM	1561	N	ALA A 197	48.785	13.822	99.214	1.00	22.10
ATOM	1562	CA	ALA A 197	48.928	12.760	100.199	1.00	24.90
ATOM	1563	CB	ALA A 197	49.627	13.307	101.437	1.00	27.83
ATOM	1564	C	ALA A 197	47.644	12.069	100.608	1.00	26.20
ATOM	1565	O	ALA A 197	46.553	12.617	100.484	1.00	22.82
ATOM	1566	N	PHE A 198	47.795	10.849	101.102	1.00	31.74
ATOM	1567	CA	PHE A 198	46.663	10.072	101.580	1.00	28.74
ATOM	1568	CB	PHE A 198	47.130	8.691	102.036	1.00	30.66
ATOM	1569	CG	PHE A 198	46.009	7.766	102.399	1.00	29.61
ATOM	1570	CD1	PHE A 198	45.496	6.879	101.463	1.00	28.76
ATOM	1571	CD2	PHE A 198	45.426	7.822	103.657	1.00	28.43
ATOM	1572	CE1	PHE A 198	44.415	6.057	101.773	1.00	35.72
ATOM	1573	CE2	PHE A 198	44.340	7.004	103.970	1.00	34.62
ATOM	1574	CZ	PHE A 198	43.837	6.121	103.029	1.00	35.73
ATOM	1575	C	PHE A 198	46.121	10.814	102.802	1.00	28.95
ATOM	1576	O	PHE A 198	46.892	11.347	103.596	1.00	25.72
ATOM	1577	N	PRO A 199	44.792	10.905	102.941	1.00	28.27
ATOM	1578	CD	PRO A 199	44.100	11.499	104.099	1.00	33.97
ATOM	1579	CA	PRO A 199	43.313	10.364	102.008	1.00	32.80
ATOM	1580	CB	PRO A 199	42.550	10.312	102.858	1.00	29.84
ATOM	1581	CG	PRO A 199	42.665	11.612	103.592	1.00	37.32
ATOM	1582	C	PRO A 199	43.773	11.476	100.965	1.00	35.02
ATOM	1583	O	PRO A 199	44.052	12.631	101.280	1.00	48.84
ATOM	1584	N	PHE A 200	43.441	11.156	99.734	1.00	33.64

141/263

Figure 18-25

ATOM	1585	CA	PHE	A	200	43.418	12.179	98.718	1.00	28.12
ATOM	1586	CB	PHE	A	200	43.927	11.579	97.411	1.00	26.69
ATOM	1587	CG	PHE	A	200	45.226	10.833	97.561	1.00	27.33
ATOM	1588	CD1	PHE	A	200	45.239	9.510	97.995	1.00	29.79
ATOM	1589	CD2	PHE	A	200	46.439	11.461	97.302	1.00	24.38
ATOM	1590	CE1	PHE	A	200	46.444	8.820	98.168	1.00	29.45
ATOM	1591	CE2	PHE	A	200	47.651	10.782	97.473	1.00	31.41
ATOM	1592	CZ	PHE	A	200	47.653	9.458	97.906	1.00	29.64
ATOM	1593	C	PHE	A	200	42.042	12.795	98.518	1.00	26.15
ATOM	1594	O	PHE	A	200	41.935	13.889	97.986	1.00	27.96
ATOM	1595	N	GLU	A	201	41.002	12.101	98.979	1.00	28.52
ATOM	1596	CA	GLU	A	201	39.614	12.534	98.806	1.00	35.04
ATOM	1597	CB	GLU	A	201	38.695	11.316	98.810	1.00	33.61
ATOM	1598	CG	GLU	A	201	39.087	10.240	97.838	1.00	37.80
ATOM	1599	CD	GLU	A	201	38.222	9.016	97.997	1.00	43.48
ATOM	1600	OE1	GLU	A	201	36.992	9.142	97.825	1.00	40.96
ATOM	1601	OE2	GLU	A	201	38.772	7.937	98.298	1.00	44.17
ATOM	1602	C	GLU	A	201	39.077	13.516	99.837	1.00	36.30
ATOM	1603	O	GLU	A	201	38.087	14.206	99.592	1.00	36.47
ATOM	1604	N	LYS	A	202	39.693	13.552	101.007	1.00	34.63
ATOM	1605	CA	LYS	A	202	39.229	14.460	102.030	1.00	34.09
ATOM	1606	CB	LYS	A	202	38.294	13.729	102.992	1.00	40.88
ATOM	1607	CG	LYS	A	202	37.011	13.318	102.292	1.00	43.17
ATOM	1608	CD	LYS	A	202	35.935	12.854	103.230	1.00	47.39
ATOM	1609	CE	LYS	A	202	34.628	12.663	102.469	1.00	47.74
ATOM	1610	NZ	LYS	A	202	33.504	12.290	103.378	1.00	53.56
ATOM	1611	C	LYS	A	202	40.382	15.101	102.753	1.00	36.27
ATOM	1612	O	LYS	A	202	41.520	14.666	102.613	1.00	28.06
ATOM	1613	N	GLY	A	203	40.080	16.152	103.509	1.00	31.91
ATOM	1614	CA	GLY	A	203	41.115	16.862	104.228	1.00	33.75
ATOM	1615	C	GLY	A	203	41.288	18.288	103.729	1.00	30.54
ATOM	1616	O	GLY	A	203	42.174	18.996	104.200	1.00	28.04
ATOM	1617	N	PHE	A	204	40.458	18.713	102.778	1.00	29.93
ATOM	1618	CA	PHE	A	204	40.557	20.077	102.260	1.00	35.76
ATOM	1619	CB	PHE	A	204	39.863	20.217	100.901	1.00	31.41
ATOM	1620	CG	PHE	A	204	40.498	19.416	99.803	1.00	31.06
ATOM	1621	CD1	PHE	A	204	40.169	18.075	99.618	1.00	35.66
ATOM	1622	CD2	PHE	A	204	41.431	20.002	98.955	1.00	30.79
ATOM	1623	CE1	PHE	A	204	40.761	17.329	98.597	1.00	35.20
ATOM	1624	CE2	PHE	A	204	42.033	19.267	97.931	1.00	36.08
ATOM	1625	CZ	PHE	A	204	41.697	17.928	97.751	1.00	36.54
ATOM	1626	C	PHE	A	204	39.967	21.103	103.231	1.00	37.30
ATOM	1627	O	PHE	A	204	39.088	20.786	104.040	1.00	33.56
ATOM	1628	N	LEU	A	205	40.451	22.337	103.128	1.00	38.52
ATOM	1629	CA	LEU	A	205	40.012	23.427	103.993	1.00	36.81
ATOM	1630	CB	LEU	A	205	40.801	24.695	103.659	1.00	34.73
ATOM	1631	CG	LEU	A	205	40.496	25.954	104.479	1.00	40.98
ATOM	1632	CD1	LEU	A	205	40.690	25.677	105.965	1.00	39.87
ATOM	1633	CD2	LEU	A	205	41.415	27.079	104.032	1.00	39.94
ATOM	1634	C	LEU	A	205	38.520	23.728	103.925	1.00	36.58
ATOM	1635	O	LEU	A	205	37.931	24.178	104.905	1.00	40.98
ATOM	1636	N	GLU	A	206	37.909	23.477	102.774	1.00	36.07
ATOM	1637	CA	GLU	A	206	36.486	23.748	102.586	1.00	36.30
ATOM	1638	CB	GLU	A	206	36.107	23.597	101.105	1.00	39.98
ATOM	1639	CG	GLU	A	206	36.890	24.473	100.131	1.00	48.04
ATOM	1640	CD	GLU	A	206	38.307	23.980	99.868	1.00	51.87
ATOM	1641	OE1	GLU	A	206	39.146	23.993	100.792	1.00	50.32
ATOM	1642	OE2	GLU	A	206	38.581	23.569	98.716	1.00	56.69
ATOM	1643	C	GLU	A	206	35.572	22.852	103.427	1.00	33.85
ATOM	1644	O	GLU	A	206	34.433	23.213	103.718	1.00	26.22
ATOM	1645	N	GLU	A	207	36.071	21.679	103.805	1.00	31.68
ATOM	1646	CA	GLU	A	207	35.297	20.726	104.599	1.00	31.65
ATOM	1647	CB	GLU	A	207	36.000	19.369	104.566	1.00	34.15
ATOM	1648	CG	GLU	A	207	36.044	18.741	103.179	1.00	33.80
ATOM	1649	CD	GLU	A	207	37.182	17.751	103.022	1.00	33.85
ATOM	1650	OE1	GLU	A	207	37.487	17.025	103.995	1.00	33.22

ATOM	1651	OE2	GLU	A	207	37.760	17.688	101.916	1.00	35.48
ATOM	1652	C	GLU	A	207	35.182	21.229	106.033	1.00	35.06
ATOM	1653	O	GLU	A	207	36.009	20.894	106.887	1.00	34.16
ATOM	1654	N	ILE	A	208	34.150	22.024	106.302	1.00	35.99
ATOM	1655	CA	ILE	A	208	33.968	22.604	107.634	1.00	38.96
ATOM	1656	CB	ILE	A	208	33.737	24.134	107.529	1.00	42.74
ATOM	1657	CG2	ILE	A	208	33.717	24.762	108.914	1.00	48.29
ATOM	1658	CG1	ILE	A	208	34.841	24.795	106.700	1.00	40.34
ATOM	1659	CD1	ILE	A	208	36.207	24.758	107.335	1.00	46.23
ATOM	1660	C	ILE	A	208	32.821	21.998	108.452	1.00	38.32
ATOM	1661	O	ILE	A	208	32.558	22.434	109.571	1.00	40.08
ATOM	1662	N	GLY	A	209	32.142	20.997	107.901	1.00	34.36
ATOM	1663	CA	GLY	A	209	31.047	20.374	108.620	1.00	33.32
ATOM	1664	C	GLY	A	209	29.699	20.673	107.993	1.00	37.87
ATOM	1665	O	GLY	A	209	29.579	21.581	107.173	1.00	40.56
ATOM	1666	N	GLU	A	210	28.676	19.917	108.380	1.00	37.38
ATOM	1667	CA	GLU	A	210	27.337	20.118	107.831	1.00	42.34
ATOM	1668	CB	GLU	A	210	27.008	19.012	106.823	1.00	42.73
ATOM	1669	CG	GLU	A	210	26.860	17.636	107.460	1.00	47.38
ATOM	1670	CD	GLU	A	210	26.633	16.532	106.443	1.00	52.68
ATOM	1671	OE1	GLU	A	210	26.385	15.379	106.860	1.00	50.59
ATOM	1672	OE2	GLU	A	210	26.711	16.810	105.226	1.00	53.78
ATOM	1673	C	GLU	A	210	26.287	20.114	108.938	1.00	42.90
ATOM	1674	O	GLU	A	210	26.516	19.577	110.022	1.00	45.94
ATOM	1675	N	GLY	A	211	25.130	20.702	108.654	1.00	43.16
ATOM	1676	CA	GLY	A	211	24.068	20.751	109.642	1.00	43.98
ATOM	1677	C	GLY	A	211	24.514	21.450	110.911	1.00	45.01
ATOM	1678	O	GLY	A	211	25.186	22.479	110.858	1.00	48.15
ATOM	1679	N	LYS	A	212	24.145	20.896	112.059	1.00	41.63
ATOM	1680	CA	LYS	A	212	24.528	21.495	113.328	1.00	45.07
ATOM	1681	CB	LYS	A	212	23.913	20.715	114.490	1.00	46.59
ATOM	1682	CG	LYS	A	212	22.386	20.591	114.462	1.00	55.31
ATOM	1683	CD	LYS	A	212	21.651	21.945	114.481	1.00	57.42
ATOM	1684	CE	LYS	A	212	21.749	22.696	113.151	1.00	59.71
ATOM	1685	NZ	LYS	A	212	21.051	24.017	113.178	1.00	57.43
ATOM	1686	C	LYS	A	212	26.046	21.513	113.469	1.00	42.08
ATOM	1687	O	LYS	A	212	26.598	22.326	114.207	1.00	40.03
ATOM	1688	N	GLY	A	213	26.713	20.615	112.751	1.00	39.51
ATOM	1689	CA	GLY	A	213	28.163	20.538	112.817	1.00	40.11
ATOM	1690	C	GLY	A	213	28.888	21.519	111.916	1.00	38.25
ATOM	1691	O	GLY	A	213	30.122	21.575	111.913	1.00	34.70
ATOM	1692	N	LYS	A	214	28.131	22.295	111.143	1.00	37.31
ATOM	1693	CA	LYS	A	214	28.736	23.274	110.250	1.00	39.58
ATOM	1694	CB	LYS	A	214	27.656	24.017	109.463	1.00	44.69
ATOM	1695	CG	LYS	A	214	28.189	25.030	108.461	1.00	44.53
ATOM	1696	CD	LYS	A	214	27.047	25.704	107.720	1.00	47.71
ATOM	1697	CE	LYS	A	214	27.553	26.759	106.754	1.00	52.94
ATOM	1698	NZ	LYS	A	214	28.453	26.183	105.717	1.00	57.45
ATOM	1699	C	LYS	A	214	29.547	24.259	111.085	1.00	40.16
ATOM	1700	O	LYS	A	214	29.002	24.963	111.933	1.00	37.92
ATOM	1701	N	GLY	A	215	30.851	24.295	110.846	1.00	36.57
ATOM	1702	CA	GLY	A	215	31.716	25.183	111.593	1.00	35.03
ATOM	1703	C	GLY	A	215	32.431	24.448	112.709	1.00	34.57
ATOM	1704	O	GLY	A	215	33.216	25.039	113.454	1.00	33.76
ATOM	1705	N	TYR	A	216	32.168	23.153	112.837	1.00	34.61
ATOM	1706	CA	TYR	A	216	32.816	22.378	113.885	1.00	35.00
ATOM	1707	CB	TYR	A	216	31.763	21.683	114.753	1.00	36.19
ATOM	1708	CG	TYR	A	216	30.928	22.671	115.547	1.00	36.68
ATOM	1709	CD1	TYR	A	216	29.961	23.462	114.925	1.00	35.83
ATOM	1710	CE1	TYR	A	216	29.249	24.431	115.641	1.00	40.89
ATOM	1711	CD2	TYR	A	216	31.163	22.869	116.910	1.00	41.50
ATOM	1712	CE2	TYR	A	216	30.459	23.834	117.634	1.00	40.69
ATOM	1713	CZ	TYR	A	216	29.505	24.612	116.994	1.00	40.17
ATOM	1714	OH	TYR	A	216	28.816	25.566	117.708	1.00	38.09
ATOM	1715	C	TYR	A	216	33.877	21.384	113.401	1.00	34.05
ATOM	1716	O	TYR	A	216	34.263	20.462	114.127	1.00	31.87

ATOM	1717	N	ASN	A	217	34.343	21.580	112.170	1.00	29.90
ATOM	1718	CA	ASN	A	217	35.398	20.748	111.606	1.00	30.02
ATOM	1719	CB	ASN	A	217	34.833	19.727	110.615	1.00	26.46
ATOM	1720	CG	ASN	A	217	35.897	18.764	110.105	1.00	30.13
ATOM	1721	OD1	ASN	A	217	36.558	19.022	109.097	1.00	29.80
ATOM	1722	ND2	ASN	A	217	36.094	17.659	110.831	1.00	19.92
ATOM	1723	C	ASN	A	217	36.378	21.686	110.915	1.00	30.23
ATOM	1724	O	ASN	A	217	35.983	22.502	110.080	1.00	27.88
ATOM	1725	N	LEU	A	218	37.655	21.577	111.271	1.00	29.45
ATOM	1726	CA	LEU	A	218	38.670	22.451	110.698	1.00	28.76
ATOM	1727	CB	LEU	A	218	39.160	23.444	111.753	1.00	29.02
ATOM	1728	CG	LEU	A	218	39.513	24.867	111.307	1.00	34.69
ATOM	1729	CD1	LEU	A	218	40.432	25.480	112.367	1.00	32.93
ATOM	1730	CD2	LEU	A	218	40.197	24.873	109.954	1.00	30.69
ATOM	1731	C	LEU	A	218	39.870	21.657	110.207	1.00	26.65
ATOM	1732	O	LEU	A	218	40.527	20.981	110.999	1.00	25.25
ATOM	1733	N	ASN	A	219	40.151	21.752	108.909	1.00	25.21
ATOM	1734	CA	ASN	A	219	41.287	21.069	108.294	1.00	21.91
ATOM	1735	CB	ASN	A	219	40.875	20.314	107.018	1.00	23.69
ATOM	1736	CG	ASN	A	219	39.972	19.144	107.298	1.00	27.88
ATOM	1737	OD1	ASN	A	219	40.153	18.440	108.289	1.00	29.28
ATOM	1738	ND2	ASN	A	219	39.018	18.900	106.407	1.00	24.48
ATOM	1739	C	ASN	A	219	42.355	22.074	107.906	1.00	23.46
ATOM	1740	O	ASN	A	219	42.059	23.073	107.259	1.00	28.17
ATOM	1741	N	ILE	A	220	43.595	21.804	108.287	1.00	23.90
ATOM	1742	CA	ILE	A	220	44.702	22.684	107.945	1.00	23.22
ATOM	1743	CB	ILE	A	220	45.468	23.131	109.212	1.00	28.73
ATOM	1744	CG2	ILE	A	220	46.601	24.078	108.831	1.00	26.01
ATOM	1745	CG1	ILE	A	220	44.502	23.783	110.212	1.00	26.36
ATOM	1746	CD1	ILE	A	220	43.771	25.004	109.688	1.00	25.74
ATOM	1747	C	ILE	A	220	45.669	21.929	107.018	1.00	25.29
ATOM	1748	O	ILE	A	220	46.631	21.315	107.477	1.00	20.44
ATOM	1749	N	PRO	A	221	45.396	21.924	105.703	1.00	26.34
ATOM	1750	CD	PRO	A	221	44.234	22.497	104.999	1.00	28.22
ATOM	1751	CA	PRO	A	221	46.271	21.234	104.747	1.00	26.92
ATOM	1752	CB	PRO	A	221	45.454	21.279	103.457	1.00	27.81
ATOM	1753	CG	PRO	A	221	44.774	22.622	103.582	1.00	30.62
ATOM	1754	C	PRO	A	221	47.595	21.977	104.625	1.00	27.45
ATOM	1755	O	PRO	A	221	47.603	23.199	104.457	1.00	31.21
ATOM	1756	N	LEU	A	222	48.704	21.242	104.703	1.00	26.01
ATOM	1757	CA	LEU	A	222	50.038	21.838	104.640	1.00	26.41
ATOM	1758	CB	LEU	A	222	50.726	21.650	105.997	1.00	26.12
ATOM	1759	CG	LEU	A	222	49.960	22.322	107.150	1.00	27.67
ATOM	1760	CD1	LEU	A	222	50.531	21.899	108.497	1.00	30.97
ATOM	1761	CD2	LEU	A	222	50.024	23.839	106.985	1.00	31.59
ATOM	1762	C	LEU	A	222	50.911	21.286	103.504	1.00	28.97
ATOM	1763	O	LEU	A	222	50.784	20.128	103.117	1.00	27.95
ATOM	1764	N	PRO	A	223	51.821	22.116	102.964	1.00	31.52
ATOM	1765	CD	PRO	A	223	52.059	23.518	103.358	1.00	29.08
ATOM	1766	CA	PRO	A	223	52.727	21.753	101.865	1.00	29.93
ATOM	1767	CB	PRO	A	223	53.265	23.109	101.428	1.00	29.16
ATOM	1768	CG	PRO	A	223	53.458	23.771	102.779	1.00	25.86
ATOM	1769	C	PRO	A	223	53.862	20.782	102.206	1.00	33.62
ATOM	1770	O	PRO	A	223	54.179	20.531	103.376	1.00	26.55
ATOM	1771	N	LYS	A	224	54.479	20.257	101.153	1.00	34.00
ATOM	1772	CA	LYS	A	224	55.595	19.320	101.264	1.00	32.88
ATOM	1773	CB	LYS	A	224	55.938	18.767	99.884	1.00	36.31
ATOM	1774	CG	LYS	A	224	54.761	18.204	99.115	1.00	39.37
ATOM	1775	CD	LYS	A	224	55.150	17.998	97.658	1.00	45.23
ATOM	1776	CE	LYS	A	224	53.989	17.478	96.835	1.00	47.90
ATOM	1777	NZ	LYS	A	224	54.331	17.441	95.388	1.00	46.60
ATOM	1778	C	LYS	A	224	56.817	20.054	101.798	1.00	29.43
ATOM	1779	O	LYS	A	224	56.933	21.270	101.640	1.00	24.10
ATOM	1780	N	GLY	A	225	57.735	19.305	102.403	1.00	25.00
ATOM	1781	CA	GLY	A	225	58.947	19.896	102.942	1.00	26.20
ATOM	1782	C	GLY	A	225	58.727	20.792	104.154	1.00	29.44

144/263

Figure 18-28

ATOM	1783	O	GLY	A	225	59.610	21.562	104.528	1.00	29.09
ATOM	1784	N	LEU	A	226	57.560	20.679	104.777	1.00	24.26
ATOM	1785	CA	LEU	A	226	57.212	21.488	105.951	1.00	25.35
ATOM	1786	CB	LEU	A	226	55.930	20.925	106.579	1.00	23.23
ATOM	1787	CG	LEU	A	226	55.172	21.757	107.611	1.00	28.28
ATOM	1788	CD1	LEU	A	226	54.596	22.972	106.911	1.00	28.07
ATOM	1789	CD2	LEU	A	226	54.036	20.933	108.226	1.00	27.49
ATOM	1790	C	LEU	A	226	58.333	21.501	106.998	1.00	24.79
ATOM	1791	O	LEU	A	226	58.902	20.450	107.299	1.00	26.15
ATOM	1792	N	ASN	A	227	58.664	22.674	107.548	1.00	23.94
ATOM	1793	CA	ASN	A	227	59.702	22.733	108.578	1.00	24.89
ATOM	1794	CB	ASN	A	227	60.751	23.823	108.269	1.00	27.43
ATOM	1795	CG	ASN	A	227	60.190	25.231	108.334	1.00	31.62
ATOM	1796	OD1	ASN	A	227	59.598	25.632	109.336	1.00	31.17
ATOM	1797	ND2	ASN	A	227	60.395	25.998	107.267	1.00	28.06
ATOM	1798	C	ASN	A	227	59.076	22.957	109.960	1.00	23.16
ATOM	1799	O	ASN	A	227	57.873	23.206	110.065	1.00	18.45
ATOM	1800	N	ASP	A	228	59.880	22.862	111.018	1.00	21.29
ATOM	1801	CA	ASP	A	228	59.357	23.032	112.375	1.00	25.80
ATOM	1802	CB	ASP	A	228	60.464	22.893	113.426	1.00	24.02
ATOM	1803	CG	ASP	A	228	61.110	21.520	113.422	1.00	26.48
ATOM	1804	OD1	ASP	A	228	60.410	20.530	113.135	1.00	29.55
ATOM	1805	OD2	ASP	A	228	62.311	21.425	113.744	1.00	29.88
ATOM	1806	C	ASP	A	228	58.628	24.341	112.620	1.00	27.83
ATOM	1807	O	ASP	A	228	57.589	24.360	113.284	1.00	25.68
ATOM	1808	N	ASN	A	229	59.167	25.437	112.098	1.00	25.78
ATOM	1809	CA	ASN	A	229	58.537	26.739	112.297	1.00	27.75
ATOM	1810	CB	ASN	A	229	59.453	27.850	111.770	1.00	32.77
ATOM	1811	CG	ASN	A	229	60.707	28.020	112.621	1.00	30.35
ATOM	1812	OD1	ASN	A	229	60.635	28.433	113.782	1.00	33.12
ATOM	1813	ND2	ASN	A	229	61.856	27.691	112.053	1.00	28.11
ATOM	1814	C	ASN	A	229	57.168	26.817	111.645	1.00	29.47
ATOM	1815	O	ASN	A	229	56.230	27.387	112.202	1.00	26.75
ATOM	1816	N	GLU	A	230	57.041	26.228	110.463	1.00	30.80
ATOM	1817	CA	GLU	A	230	55.761	26.244	109.773	1.00	30.77
ATOM	1818	CB	GLU	A	230	55.929	25.716	108.341	1.00	29.11
ATOM	1819	CG	GLU	A	230	56.897	26.531	107.507	1.00	35.94
ATOM	1820	CD	GLU	A	230	57.119	25.946	106.125	1.00	37.77
ATOM	1821	OE1	GLU	A	230	57.465	24.748	106.039	1.00	38.98
ATOM	1822	OE2	GLU	A	230	56.957	26.684	105.129	1.00	31.32
ATOM	1823	C	GLU	A	230	54.723	25.407	110.527	1.00	30.13
ATOM	1824	O	GLU	A	230	53.563	25.799	110.631	1.00	28.35
ATOM	1825	N	PHE	A	231	55.141	24.262	111.060	1.00	32.49
ATOM	1826	CA	PHE	A	231	54.223	23.386	111.790	1.00	28.54
ATOM	1827	CB	PHE	A	231	54.913	22.075	112.191	1.00	31.22
ATOM	1828	CG	PHE	A	231	53.974	21.050	112.781	1.00	28.41
ATOM	1829	CD1	PHE	A	231	53.026	20.417	111.982	1.00	29.66
ATOM	1830	CD2	PHE	A	231	54.036	20.723	114.130	1.00	28.38
ATOM	1831	CE1	PHE	A	231	52.153	19.469	112.518	1.00	25.79
ATOM	1832	CE2	PHE	A	231	53.166	19.774	114.681	1.00	31.40
ATOM	1833	CZ	PHE	A	231	52.223	19.146	113.870	1.00	30.51
ATOM	1834	C	PHE	A	231	53.693	24.065	113.045	1.00	26.85
ATOM	1835	O	PHE	A	231	52.483	24.092	113.277	1.00	25.99
ATOM	1836	N	LEU	A	232	54.598	24.607	113.858	1.00	26.75
ATOM	1837	CA	LEU	A	232	54.193	25.283	115.092	1.00	27.25
ATOM	1838	CB	LEU	A	232	55.422	25.617	115.933	1.00	25.15
ATOM	1839	CG	LEU	A	232	56.176	24.372	116.420	1.00	28.11
ATOM	1840	CD1	LEU	A	232	57.440	24.783	117.162	1.00	27.32
ATOM	1841	CD2	LEU	A	232	55.268	23.540	117.328	1.00	27.87
ATOM	1842	C	LEU	A	232	53.371	26.542	114.800	1.00	26.98
ATOM	1843	O	LEU	A	232	52.449	26.866	115.544	1.00	23.34
ATOM	1844	N	PHE	A	233	53.694	27.232	113.708	1.00	24.99
ATOM	1845	CA	PHE	A	233	52.950	28.426	113.312	1.00	28.13
ATOM	1846	CB	PHE	A	233	53.542	29.029	112.029	1.00	30.77
ATOM	1847	CG	PHE	A	233	52.719	30.151	111.448	1.00	29.65
ATOM	1848	CD1	PHE	A	233	52.803	31.441	111.962	1.00	32.80

145/263

Figure 18-29

ATOM	1849	CD2	PHE	A	233	51.825	29.903	110.412	1.00	31.59
ATOM	1850	CE1	PHE	A	233	52.008	32.468	111.452	1.00	33.90
ATOM	1851	CE2	PHE	A	233	51.022	30.924	109.895	1.00	32.47
ATOM	1852	CZ	PHE	A	233	51.114	32.208	110.415	1.00	32.50
ATOM	1853	C	PHE	A	233	51.510	27.999	113.031	1.00	31.62
ATOM	1854	O	PHE	A	233	50.553	28.603	113.532	1.00	25.88
ATOM	1855	N	ALA	A	234	51.370	26.955	112.215	1.00	28.12
ATOM	1856	CA	ALA	A	234	50.056	26.436	111.853	1.00	25.68
ATOM	1857	CB	ALA	A	234	50.195	25.279	110.864	1.00	20.08
ATOM	1858	C	ALA	A	234	49.304	25.969	113.089	1.00	25.17
ATOM	1859	O	ALA	A	234	48.114	26.228	113.234	1.00	25.21
ATOM	1860	N	LEU	A	235	50.002	25.285	113.987	1.00	28.18
ATOM	1861	CA	LEU	A	235	49.367	24.781	115.195	1.00	33.70
ATOM	1862	CB	LEU	A	235	50.356	23.964	116.026	1.00	32.70
ATOM	1863	CG	LEU	A	235	49.772	22.788	116.820	1.00	36.89
ATOM	1864	CD1	LEU	A	235	50.634	22.545	118.052	1.00	31.37
ATOM	1865	CD2	LEU	A	235	48.344	23.072	117.231	1.00	31.47
ATOM	1866	C	LEU	A	235	48.841	25.925	116.062	1.00	33.38
ATOM	1867	O	LEU	A	235	47.673	25.926	116.455	1.00	28.13
ATOM	1868	N	GLU	A	236	49.710	26.888	116.362	1.00	34.02
ATOM	1869	CA	GLU	A	236	49.336	28.026	117.199	1.00	37.30
ATOM	1870	CB	GLU	A	236	50.528	28.972	117.400	1.00	41.51
ATOM	1871	CG	GLU	A	236	51.675	28.356	118.188	1.00	49.54
ATOM	1872	CD	GLU	A	236	52.811	29.334	118.451	1.00	55.02
ATOM	1873	OE1	GLU	A	236	53.781	28.947	119.140	1.00	56.19
ATOM	1874	OE2	GLU	A	236	52.735	30.486	117.968	1.00	54.84
ATOM	1875	C	GLU	A	236	48.163	28.803	116.638	1.00	33.98
ATOM	1876	O	GLU	A	236	47.211	29.098	117.362	1.00	37.01
ATOM	1877	N	LYS	A	237	48.223	29.137	115.354	1.00	33.94
ATOM	1878	CA	LYS	A	237	47.140	29.888	114.726	1.00	33.10
ATOM	1879	CB	LYS	A	237	47.505	30.244	113.281	1.00	36.08
ATOM	1880	CG	LYS	A	237	48.695	31.186	113.165	1.00	33.62
ATOM	1881	CD	LYS	A	237	48.395	32.508	113.856	1.00	37.99
ATOM	1882	CE	LYS	A	237	49.569	33.471	113.762	1.00	45.24
ATOM	1883	NZ	LYS	A	237	49.285	34.737	114.500	1.00	43.49
ATOM	1884	C	LYS	A	237	45.820	29.128	114.751	1.00	31.40
ATOM	1885	O	LYS	A	237	44.793	29.680	115.131	1.00	31.67
ATOM	1886	N	SER	A	238	45.841	27.861	114.354	1.00	28.72
ATOM	1887	CA	SER	A	238	44.610	27.080	114.335	1.00	31.74
ATOM	1888	CB	SER	A	238	44.834	25.720	113.660	1.00	28.90
ATOM	1889	OG	SER	A	238	45.760	24.924	114.372	1.00	25.18
ATOM	1890	C	SER	A	238	44.041	26.891	115.740	1.00	33.23
ATOM	1891	O	SER	A	238	42.823	26.875	115.916	1.00	34.79
ATOM	1892	N	LEU	A	239	44.907	26.742	116.741	1.00	35.27
ATOM	1893	CA	LEU	A	239	44.413	26.587	118.108	1.00	37.57
ATOM	1894	CB	LEU	A	239	45.554	26.307	119.090	1.00	38.58
ATOM	1895	CG	LEU	A	239	46.176	24.907	119.038	1.00	39.74
ATOM	1896	CD1	LEU	A	239	47.276	24.797	120.075	1.00	35.82
ATOM	1897	CD2	LEU	A	239	45.109	23.861	119.301	1.00	34.93
ATOM	1898	C	LEU	A	239	43.670	27.852	118.521	1.00	39.09
ATOM	1899	O	LEU	A	239	42.628	27.782	119.174	1.00	35.50
ATOM	1900	N	GLU	A	240	44.202	29.007	118.131	1.00	39.27
ATOM	1901	CA	GLU	A	240	43.561	30.281	118.450	1.00	40.15
ATOM	1902	CB	GLU	A	240	44.366	31.448	117.883	1.00	40.42
ATOM	1903	CG	GLU	A	240	45.661	31.747	118.602	1.00	43.91
ATOM	1904	CD	GLU	A	240	46.407	32.884	117.942	1.00	49.31
ATOM	1905	OE1	GLU	A	240	45.772	33.925	117.665	1.00	49.00
ATOM	1906	OE2	GLU	A	240	47.624	32.745	117.705	1.00	54.05
ATOM	1907	C	GLU	A	240	42.165	30.312	117.849	1.00	39.58
ATOM	1908	O	GLU	A	240	41.224	30.822	118.455	1.00	40.99
ATOM	1909	N	ILE	A	241	42.039	29.764	116.645	1.00	35.70
ATOM	1910	CA	ILE	A	241	40.754	29.726	115.964	1.00	38.23
ATOM	1911	CB	ILE	A	241	40.904	29.150	114.546	1.00	37.55
ATOM	1912	CG2	ILE	A	241	39.535	29.005	113.895	1.00	37.30
ATOM	1913	CG1	ILE	A	241	41.832	30.048	113.724	1.00	38.36
ATOM	1914	CD1	ILE	A	241	42.106	29.541	112.320	1.00	36.15

146/263 Figure 18-30

ATOM	1915	C	ILE A 241	39.751	28.881	116.737	1.00	37.31
ATOM	1916	O	ILE A 241	38.591	29.264	116.884	1.00	37.91
ATOM	1917	N	VAL A 242	40.203	27.732	117.231	1.00	37.07
ATOM	1918	CA	VAL A 242	39.336	26.832	117.981	1.00	38.35
ATOM	1919	CB	VAL A 242	40.025	25.477	118.250	1.00	37.58
ATOM	1920	CG1	VAL A 242	39.120	24.581	119.078	1.00	31.91
ATOM	1921	CG2	VAL A 242	40.364	24.803	116.928	1.00	39.21
ATOM	1922	C	VAL A 242	38.930	27.451	119.305	1.00	40.40
ATOM	1923	O	VAL A 242	37.759	27.422	119.675	1.00	38.19
ATOM	1924	N	LYS A 243	39.905	28.008	120.014	1.00	45.47
ATOM	1925	CA	LYS A 243	39.661	28.654	121.301	1.00	48.74
ATOM	1926	CB	LYS A 243	40.945	29.319	121.801	1.00	51.01
ATOM	1927	CG	LYS A 243	41.853	28.426	122.614	1.00	56.09
ATOM	1928	CD	LYS A 243	41.250	28.149	123.991	1.00	57.39
ATOM	1929	CE	LYS A 243	41.054	29.436	124.783	1.00	59.53
ATOM	1930	NZ	LYS A 243	40.448	29.193	126.127	1.00	57.91
ATOM	1931	C	LYS A 243	38.559	29.705	121.260	1.00	51.67
ATOM	1932	O	LYS A 243	37.815	29.871	122.226	1.00	52.84
ATOM	1933	N	GLU A 244	38.451	30.410	120.140	1.00	53.77
ATOM	1934	CA	GLU A 244	37.460	31.471	120.004	1.00	54.74
ATOM	1935	CB	GLU A 244	37.954	32.497	118.986	1.00	55.15
ATOM	1936	CG	GLU A 244	37.068	33.717	118.865	1.00	60.63
ATOM	1937	CD	GLU A 244	37.602	34.714	117.868	1.00	65.87
ATOM	1938	OE1	GLU A 244	38.746	35.181	118.053	1.00	70.36
ATOM	1939	OE2	GLU A 244	36.879	35.031	116.900	1.00	67.09
ATOM	1940	C	GLU A 244	36.051	31.025	119.626	1.00	52.65
ATOM	1941	O	GLU A 244	35.127	31.838	119.606	1.00	55.59
ATOM	1942	N	VAL A 245	35.869	29.745	119.332	1.00	50.57
ATOM	1943	CA	VAL A 245	34.546	29.269	118.947	1.00	45.75
ATOM	1944	CB	VAL A 245	34.475	29.081	117.409	1.00	46.91
ATOM	1945	CG1	VAL A 245	33.085	28.634	116.986	1.00	52.62
ATOM	1946	CG2	VAL A 245	34.825	30.389	116.716	1.00	48.34
ATOM	1947	C	VAL A 245	34.130	27.969	119.642	1.00	42.67
ATOM	1948	O	VAL A 245	33.021	27.480	119.445	1.00	43.61
ATOM	1949	N	PHE A 246	35.001	27.417	120.477	1.00	40.87
ATOM	1950	CA	PHE A 246	34.662	26.168	121.139	1.00	37.47
ATOM	1951	CB	PHE A 246	35.106	24.991	120.257	1.00	37.00
ATOM	1952	CG	PHE A 246	34.450	23.685	120.604	1.00	33.22
ATOM	1953	CD1	PHE A 246	33.111	23.467	120.302	1.00	33.93
ATOM	1954	CD2	PHE A 246	35.168	22.674	121.234	1.00	32.13
ATOM	1955	OE1	PHE A 246	32.493	22.260	120.621	1.00	37.75
ATOM	1956	OE2	PHE A 246	34.561	21.459	121.561	1.00	35.92
ATOM	1957	CE	PHE A 246	33.217	21.252	121.251	1.00	36.30
ATOM	1958	C	PHE A 246	35.322	26.065	122.509	1.00	38.93
ATOM	1959	O	PHE A 246	36.546	26.158	122.630	1.00	40.66
ATOM	1960	N	GLU A 247	34.500	25.870	123.537	1.00	38.59
ATOM	1961	CA	GLU A 247	34.970	25.733	124.918	1.00	44.60
ATOM	1962	CB	GLU A 247	34.146	25.615	125.865	1.00	47.07
ATOM	1963	CG	GLU A 247	33.161	27.569	125.185	1.00	56.16
ATOM	1964	CD	GLU A 247	31.944	26.865	124.577	1.00	62.03
ATOM	1965	OE1	GLU A 247	32.096	26.088	123.607	1.00	61.85
ATOM	1966	OE2	GLU A 247	30.822	27.094	125.083	1.00	64.59
ATOM	1967	C	GLU A 247	34.774	24.269	125.285	1.00	39.40
ATOM	1968	O	GLU A 247	33.727	23.879	125.794	1.00	39.91
ATOM	1969	N	PRO A 248	35.792	23.442	125.041	1.00	38.64
ATOM	1970	CD	PRO A 248	37.101	23.817	124.483	1.00	33.25
ATOM	1971	CA	PRO A 248	35.769	22.006	125.316	1.00	35.84
ATOM	1972	CB	PRO A 248	37.047	21.531	124.648	1.00	36.05
ATOM	1973	CG	PRO A 248	37.970	22.687	124.982	1.00	34.21
ATOM	1974	C	PRO A 248	35.736	21.611	126.779	1.00	33.94
ATOM	1975	O	PRO A 248	36.445	22.186	127.597	1.00	32.05
ATOM	1976	N	GLU A 249	34.914	20.616	127.096	1.00	29.39
ATOM	1977	CA	GLU A 249	34.841	20.105	128.459	1.00	33.12
ATOM	1978	CB	GLU A 249	33.521	19.361	128.693	1.00	30.36
ATOM	1979	CG	GLU A 249	32.284	20.212	128.564	1.00	35.98
ATOM	1980	CD	GLU A 249	31.026	19.388	128.668	1.00	40.52

147/263

Figure 18-31

ATOM	1981	OE1	GLU	A	249	30.817	18.509	127.804	1.00	40.27
ATOM	1982	OE2	GLU	A	249	30.252	19.609	129.620	1.00	38.57
ATOM	1983	C	GLU	A	249	35.995	19.119	128.623	1.00	32.30
ATOM	1984	O	GLU	A	249	36.472	18.884	129.728	1.00	28.51
ATOM	1985	N	VAL	A	250	36.434	18.547	127.502	1.00	33.74
ATOM	1986	CA	VAL	A	250	37.516	17.563	127.494	1.00	29.31
ATOM	1987	CB	VAL	A	250	36.988	16.174	127.926	1.00	29.85
ATOM	1988	CG1	VAL	A	250	35.908	15.711	126.958	1.00	24.36
ATOM	1989	CG2	VAL	A	250	38.121	15.166	127.978	1.00	25.60
ATOM	1990	C	VAL	A	250	38.066	17.453	126.076	1.00	29.30
ATOM	1991	O	VAL	A	250	37.358	17.741	125.114	1.00	24.46
ATOM	1992	N	TYR	A	251	39.323	17.046	125.930	1.00	27.96
ATOM	1993	CA	TYR	A	251	39.865	16.913	124.585	1.00	30.06
ATOM	1994	CB	TYR	A	251	40.585	18.206	124.165	1.00	25.89
ATOM	1995	CG	TYR	A	251	41.998	18.370	124.692	1.00	29.90
ATOM	1996	CD1	TYR	A	251	43.087	17.794	124.029	1.00	26.02
ATOM	1997	CE1	TYR	A	251	44.390	17.953	124.507	1.00	29.20
ATOM	1998	CD2	TYR	A	251	42.249	19.107	125.849	1.00	31.96
ATOM	1999	CE2	TYR	A	251	43.551	19.271	126.338	1.00	31.54
ATOM	2000	CZ	TYR	A	251	44.614	18.694	125.664	1.00	31.46
ATOM	2001	OH	TYR	A	251	45.894	18.854	126.152	1.00	29.69
ATOM	2002	C	TYR	A	251	40.801	15.731	124.451	1.00	27.56
ATOM	2003	O	TYR	A	251	41.382	15.273	125.436	1.00	28.23
ATOM	2004	N	LEU	A	252	40.908	15.222	123.227	1.00	23.52
ATOM	2005	CA	LEU	A	252	41.806	14.117	122.919	1.00	26.53
ATOM	2006	CB	LEU	A	252	41.057	12.930	122.293	1.00	25.74
ATOM	2007	CG	LEU	A	252	40.266	12.001	123.221	1.00	28.49
ATOM	2008	CD1	LEU	A	252	39.122	12.753	123.868	1.00	27.67
ATOM	2009	CD2	LEU	A	252	39.727	10.835	122.414	1.00	32.00
ATOM	2010	C	LEU	A	252	42.842	14.638	121.932	1.00	27.53
ATOM	2011	O	LEU	A	252	42.528	15.444	121.055	1.00	24.42
ATOM	2012	N	LEU	A	253	44.075	14.176	122.078	1.00	24.60
ATOM	2013	CA	LEU	A	253	45.157	14.599	121.204	1.00	25.04
ATOM	2014	CB	LEU	A	253	46.176	15.400	122.017	1.00	22.48
ATOM	2015	CG	LEU	A	253	47.456	15.880	121.323	1.00	21.05
ATOM	2016	CD1	LEU	A	253	47.105	16.833	120.175	1.00	23.05
ATOM	2017	CD2	LEU	A	253	48.348	16.578	122.360	1.00	16.40
ATOM	2018	C	LEU	A	253	45.822	13.374	120.580	1.00	23.55
ATOM	2019	O	LEU	A	253	46.329	12.516	121.303	1.00	22.11
ATOM	2020	N	GLN	A	254	45.811	13.287	119.248	1.00	22.33
ATOM	2021	CA	GLN	A	254	46.417	12.150	118.552	1.00	19.84
ATOM	2022	CB	GLN	A	254	45.542	11.731	117.348	1.00	23.09
ATOM	2023	CG	GLN	A	254	46.075	12.038	115.963	1.00	35.49
ATOM	2024	CD	GLN	A	254	47.073	11.017	115.453	1.00	31.26
ATOM	2025	OE1	GLN	A	254	46.712	9.937	114.961	1.00	33.69
ATOM	2026	NE2	GLN	A	254	48.338	11.349	115.574	1.00	31.02
ATOM	2027	C	GLN	A	254	47.831	12.576	118.153	1.00	22.46
ATOM	2028	O	GLN	A	254	48.034	13.599	117.478	1.00	17.56
ATOM	2029	N	LEU	A	255	48.804	11.781	118.590	1.00	17.64
ATOM	2030	CA	LEU	A	255	50.213	12.079	118.383	1.00	17.04
ATOM	2031	CB	LEU	A	255	50.894	12.136	119.750	1.00	14.75
ATOM	2032	CG	LEU	A	255	50.277	13.196	120.670	1.00	25.02
ATOM	2033	CD1	LEU	A	255	50.732	12.996	122.107	1.00	21.99
ATOM	2034	CD2	LEU	A	255	50.636	14.578	120.149	1.00	18.30
ATOM	2035	C	LEU	A	255	51.023	11.169	117.476	1.00	21.34
ATOM	2036	O	LEU	A	255	52.089	10.705	117.875	1.00	18.73
ATOM	2037	N	GLY	A	256	50.543	10.928	116.259	1.00	22.75
ATOM	2038	CA	GLY	A	256	51.291	10.093	115.330	1.00	24.09
ATOM	2039	C	GLY	A	256	52.660	10.721	115.126	1.00	24.27
ATOM	2040	O	GLY	A	256	52.805	11.945	115.134	1.00	19.15
ATOM	2041	N	THR	A	257	53.680	9.903	114.948	1.00	24.14
ATOM	2042	CA	THR	A	257	55.014	10.440	114.765	1.00	21.32
ATOM	2043	CB	THR	A	257	56.048	9.582	115.511	1.00	17.24
ATOM	2044	OG1	THR	A	257	56.009	8.248	115.004	1.00	17.48
ATOM	2045	CG2	THR	A	257	55.728	9.532	117.016	1.00	15.73
ATOM	2046	C	THR	A	257	55.403	10.527	113.290	1.00	22.98

148/263

Figure 18-32

ATOM	2047	O	THR	A	257	56.517	10.941	112.974	1.00	20.39
ATOM	2048	N	ASP	A	258	54.493	10.177	112.379	1.00	22.20
ATOM	2049	CA	ASP	A	258	54.863	10.229	110.961	1.00	26.56
ATOM	2050	CB	ASP	A	258	53.849	9.496	110.056	1.00	25.06
ATOM	2051	CG	ASP	A	258	52.415	9.944	110.252	1.00	29.08
ATOM	2052	C	ASP	A	258	55.222	11.596	110.364	1.00	27.87
ATOM	2053	O	ASP	A	258	55.756	11.661	109.254	1.00	25.61
ATOM	2054	OD1	ASP	A	258	52.173	11.070	110.742	1.00	29.86
ATOM	2055	OD2	ASP	A	258	51.513	9.168	109.869	1.00	33.25
ATOM	2056	N	PRO	A	259	54.884	12.710	111.045	1.00	31.06
ATOM	2057	CD	PRO	A	259	54.019	12.928	112.220	1.00	28.59
ATOM	2058	CA	PRO	A	259	55.268	14.006	110.469	1.00	30.95
ATOM	2059	CB	PRO	A	259	54.447	14.993	111.296	1.00	35.06
ATOM	2060	CG	PRO	A	259	54.418	14.320	112.636	1.00	35.26
ATOM	2061	C	PRO	A	259	56.790	14.268	110.583	1.00	29.06
ATOM	2062	O	PRO	A	259	57.300	15.251	110.044	1.00	29.70
ATOM	2063	N	LEU	A	260	57.508	13.389	111.280	1.00	22.68
ATOM	2064	CA	LEU	A	260	58.960	13.545	111.455	1.00	28.41
ATOM	2065	CB	LEU	A	260	59.461	12.576	112.533	1.00	22.47
ATOM	2066	CG	LEU	A	260	58.970	12.791	113.969	1.00	20.14
ATOM	2067	CD1	LEU	A	260	59.352	11.599	114.826	1.00	22.83
ATOM	2068	CD2	LEU	A	260	59.592	14.079	114.532	1.00	20.48
ATOM	2069	C	LEU	A	260	59.770	13.344	110.160	1.00	27.95
ATOM	2070	O	LEU	A	260	59.407	12.535	109.299	1.00	27.03
ATOM	2071	N	LEU	A	261	60.874	14.081	110.040	1.00	26.76
ATOM	2072	CA	LEU	A	261	61.742	14.010	108.865	1.00	26.56
ATOM	2073	CB	LEU	A	261	63.067	14.737	109.137	1.00	23.06
ATOM	2074	CG	LEU	A	261	64.131	14.615	108.025	1.00	29.52
ATOM	2075	CD1	LEU	A	261	63.642	15.325	106.770	1.00	22.68
ATOM	2076	CD2	LEU	A	261	65.460	15.219	108.475	1.00	26.71
ATOM	2077	C	LEU	A	261	62.063	12.577	108.443	1.00	28.23
ATOM	2078	O	LEU	A	261	61.880	12.198	107.289	1.00	26.52
ATOM	2079	N	GLU	A	262	62.539	11.787	109.397	1.00	28.70
ATOM	2080	CA	GLU	A	262	62.938	10.416	109.135	1.00	31.76
ATOM	2081	CB	GLU	A	262	63.685	9.855	110.351	1.00	29.72
ATOM	2082	CG	GLU	A	262	64.890	10.683	110.803	1.00	31.33
ATOM	2083	CD	GLU	A	262	64.521	11.847	111.708	1.00	28.07
ATOM	2084	OE1	GLU	A	262	63.324	12.195	111.789	1.00	28.75
ATOM	2085	OE2	GLU	A	262	65.433	12.424	112.340	1.00	26.08
ATOM	2086	C	GLU	A	262	61.847	9.429	108.721	1.00	28.63
ATOM	2087	O	GLU	A	262	62.158	8.305	108.350	1.00	29.72
ATOM	2088	N	ASP	A	263	60.582	9.825	108.785	1.00	28.07
ATOM	2089	CA	ASP	A	263	59.513	8.902	108.412	1.00	26.85
ATOM	2090	CB	ASP	A	263	58.305	9.099	109.333	1.00	25.26
ATOM	2091	CG	ASP	A	263	57.261	7.998	109.185	1.00	33.14
ATOM	2092	OD1	ASP	A	263	56.638	7.636	110.200	1.00	29.91
ATOM	2093	OD2	ASP	A	263	57.042	7.509	108.051	1.00	26.56
ATOM	2094	C	ASP	A	263	59.150	9.146	106.957	1.00	29.44
ATOM	2095	O	ASP	A	263	58.740	10.247	106.594	1.00	24.70
ATOM	2096	N	TYR	A	264	59.303	8.111	106.130	1.00	27.51
ATOM	2097	CA	TYR	A	264	59.031	8.219	104.696	1.00	33.89
ATOM	2098	CB	TYR	A	264	59.576	7.008	103.935	1.00	40.44
ATOM	2099	CG	TYR	A	264	61.059	6.771	104.092	1.00	50.64
ATOM	2100	CD1	TYR	A	264	61.565	6.087	105.199	1.00	54.67
ATOM	2101	CE1	TYR	A	264	62.933	5.876	105.351	1.00	55.28
ATOM	2102	CD2	TYR	A	264	61.960	7.242	103.140	1.00	53.79
ATOM	2103	CE2	TYR	A	264	63.329	7.038	103.282	1.00	56.61
ATOM	2104	CZ	TYR	A	264	63.809	6.354	104.388	1.00	56.22
ATOM	2105	OH	TYR	A	264	65.161	6.147	104.524	1.00	55.90
ATOM	2106	C	TYR	A	264	57.561	8.394	104.294	1.00	31.33
ATOM	2107	O	TYR	A	264	57.311	8.825	103.178	1.00	27.15
ATOM	2108	N	LEU	A	265	56.641	8.059	105.172	1.00	26.88
ATOM	2109	CA	LEU	A	265	55.244	8.209	104.792	1.00	24.39
ATOM	2110	CB	LEU	A	265	54.360	7.189	105.527	1.00	26.55
ATOM	2111	CG	LEU	A	265	54.663	5.724	105.168	1.00	29.80
ATOM	2112	CD1	LEU	A	265	53.464	4.836	105.503	1.00	21.17

ATOM	2113	CD2	LEU	A	265	54.931	5.620	103.682	1.00	33.35
ATOM	2114	C	LEU	A	265	54.669	9.617	104.921	1.00	20.81
ATOM	2115	O	LEU	A	265	53.457	9.796	104.979	1.00	21.30
ATOM	2116	N	SER	A	266	55.540	10.622	104.959	1.00	23.23
ATOM	2117	CA	SER	A	266	55.084	12.011	105.008	1.00	26.30
ATOM	2118	CB	SER	A	266	54.856	12.502	106.444	1.00	25.16
ATOM	2119	OG	SER	A	266	56.074	12.845	107.084	1.00	22.92
ATOM	2120	C	SER	A	266	56.147	12.879	104.355	1.00	30.17
ATOM	2121	O	SER	A	266	57.334	12.555	104.385	1.00	31.65
ATOM	2122	N	LYS	A	267	55.731	13.985	103.757	1.00	31.56
ATOM	2123	CA	LYS	A	267	56.696	14.873	103.140	1.00	27.65
ATOM	2124	CB	LYS	A	267	56.140	15.425	101.834	1.00	30.54
ATOM	2125	CG	LYS	A	267	55.815	14.327	100.819	1.00	34.13
ATOM	2126	CD	LYS	A	267	57.039	13.463	100.549	1.00	29.09
ATOM	2127	CE	LYS	A	267	56.745	12.376	99.524	1.00	37.61
ATOM	2128	NZ	LYS	A	267	57.956	11.541	99.272	1.00	31.91
ATOM	2129	C	LYS	A	267	57.050	16.004	104.107	1.00	30.85
ATOM	2130	O	LYS	A	267	57.624	17.017	103.707	1.00	27.86
ATOM	2131	N	PHE	A	268	56.688	15.826	105.377	1.00	24.19
ATOM	2132	CA	PHE	A	268	57.009	16.808	106.412	1.00	25.34
ATOM	2133	CB	PHE	A	268	56.014	16.730	107.579	1.00	24.54
ATOM	2134	CG	PHE	A	268	54.636	17.256	107.257	1.00	21.68
ATOM	2135	CD1	PHE	A	268	53.631	17.221	108.216	1.00	28.65
ATOM	2136	CD2	PHE	A	268	54.346	17.806	106.011	1.00	25.14
ATOM	2137	CE1	PHE	A	268	52.357	17.728	107.944	1.00	25.34
ATOM	2138	CE2	PHE	A	268	53.077	18.315	105.730	1.00	23.79
ATOM	2139	CZ	PHE	A	268	52.082	18.275	106.702	1.00	28.13
ATOM	2140	C	PHE	A	268	58.410	16.470	106.908	1.00	25.66
ATOM	2141	O	PHE	A	268	58.778	15.299	106.994	1.00	28.44
ATOM	2142	N	ASN	A	269	59.194	17.490	107.230	1.00	25.81
ATOM	2143	CA	ASN	A	269	60.555	17.270	107.709	1.00	30.60
ATOM	2144	CB	ASN	A	269	61.566	17.938	106.767	1.00	31.97
ATOM	2145	CG	ASN	A	269	61.392	17.513	105.317	1.00	35.83
ATOM	2146	OD1	ASN	A	269	61.235	16.332	105.020	1.00	33.93
ATOM	2147	ND2	ASN	A	269	61.446	18.477	104.405	1.00	33.95
ATOM	2148	C	ASN	A	269	60.723	17.843	109.110	1.00	31.80
ATOM	2149	O	ASN	A	269	61.609	18.665	109.348	1.00	28.13
ATOM	2150	N	LEU	A	270	59.888	17.397	110.043	1.00	29.70
ATOM	2151	CA	LEU	A	270	59.954	17.918	111.406	1.00	26.87
ATOM	2152	CB	LEU	A	270	58.575	17.833	112.074	1.00	26.60
ATOM	2153	CG	LEU	A	270	57.392	18.425	111.297	1.00	29.62
ATOM	2154	CD1	LEU	A	270	56.177	18.494	112.222	1.00	28.54
ATOM	2155	CD2	LEU	A	270	57.740	19.825	110.790	1.00	29.40
ATOM	2156	C	LEU	A	270	60.979	17.242	112.301	1.00	26.83
ATOM	2157	O	LEU	A	270	61.490	16.158	111.990	1.00	19.60
ATOM	2158	N	SER	A	271	61.275	17.896	113.420	1.00	21.66
ATOM	2159	CA	SER	A	271	62.220	17.365	114.393	1.00	27.08
ATOM	2160	CB	SER	A	271	63.189	18.460	114.846	1.00	24.64
ATOM	2161	OG	SER	A	271	62.499	19.433	115.626	1.00	18.60
ATOM	2162	C	SER	A	271	61.454	16.868	115.618	1.00	23.70
ATOM	2163	O	SER	A	271	60.272	17.150	115.772	1.00	22.56
ATOM	2164	N	ASN	A	272	62.157	16.129	116.470	1.00	28.35
ATOM	2165	CA	ASN	A	272	61.649	15.593	117.739	1.00	31.03
ATOM	2166	CB	ASN	A	272	62.774	14.880	118.498	1.00	28.80
ATOM	2167	CG	ASN	A	272	62.854	13.428	118.180	1.00	36.65
ATOM	2168	OD1	ASN	A	272	63.712	12.709	118.705	1.00	29.89
ATOM	2169	ND2	ASN	A	272	61.953	12.969	117.319	1.00	40.80
ATOM	2170	C	ASN	A	272	61.167	16.695	118.661	1.00	31.83
ATOM	2171	O	ASN	A	272	60.090	16.618	119.261	1.00	27.50
ATOM	2172	N	VAL	A	273	62.032	17.693	118.804	1.00	31.49
ATOM	2173	CA	VAL	A	273	61.802	18.837	119.667	1.00	31.58
ATOM	2174	CB	VAL	A	273	63.069	19.709	119.725	1.00	35.80
ATOM	2175	CG1	VAL	A	273	62.804	20.988	120.500	1.00	48.07
ATOM	2176	CG2	VAL	A	273	64.198	18.914	120.381	1.00	42.81
ATOM	2177	C	VAL	A	273	60.608	19.665	119.234	1.00	30.13
ATOM	2178	O	VAL	A	273	59.872	20.174	120.072	1.00	31.44

150/263

Figure 18-34

ATOM	2179	N	ALA A 274	60.405	19.800	117.929	1.00	24.15
ATOM	2180	CA	ALA A 274	59.258	20.558	117.455	1.00	26.27
ATOM	2181	CB	ALA A 274	59.341	20.780	115.965	1.00	21.85
ATOM	2182	C	ALA A 274	58.005	19.759	117.789	1.00	25.68
ATOM	2183	O	ALA A 274	56.961	20.324	118.132	1.00	23.76
ATOM	2184	N	PHE A 275	58.122	18.438	117.680	1.00	25.20
ATOM	2185	CA	PHE A 275	57.015	17.538	117.974	1.00	25.89
ATOM	2186	CB	PHE A 275	57.449	16.092	117.710	1.00	25.21
ATOM	2187	CG	PHE A 275	56.340	15.088	117.870	1.00	28.85
ATOM	2188	CD1	PHE A 275	55.278	15.064	116.982	1.00	32.60
ATOM	2189	CD2	PHE A 275	56.365	14.166	118.910	1.00	28.93
ATOM	2190	CE1	PHE A 275	54.248	14.132	117.119	1.00	33.75
ATOM	2191	CE2	PHE A 275	55.343	13.231	119.059	1.00	30.83
ATOM	2192	CZ	PHE A 275	54.282	13.214	118.160	1.00	34.19
ATOM	2193	C	PHE A 275	56.607	17.712	119.445	1.00	24.63
ATOM	2194	O	PHE A 275	55.428	17.877	119.767	1.00	22.40
ATOM	2195	N	LEU A 276	57.594	17.673	120.331	1.00	25.45
ATOM	2196	CA	LEU A 276	57.357	17.837	121.766	1.00	27.94
ATOM	2197	CB	LEU A 276	58.667	17.692	122.534	1.00	26.11
ATOM	2198	CG	LEU A 276	58.651	18.132	124.001	1.00	31.15
ATOM	2199	CD1	LEU A 276	57.609	17.351	124.761	1.00	29.37
ATOM	2200	CD2	LEU A 276	60.033	17.937	124.612	1.00	27.98
ATOM	2201	C	LEU A 276	56.770	19.208	122.058	1.00	30.12
ATOM	2202	O	LEU A 276	55.822	19.348	122.838	1.00	28.69
ATOM	2203	N	LYS A 277	57.353	20.219	121.425	1.00	30.99
ATOM	2204	CA	LYS A 277	56.913	21.593	121.603	1.00	27.04
ATOM	2205	CB	LYS A 277	57.742	22.516	120.704	1.00	30.38
ATOM	2206	CG	LYS A 277	57.941	23.934	121.237	1.00	36.46
ATOM	2207	CD	LYS A 277	56.633	24.668	121.454	1.00	42.73
ATOM	2208	CE	LYS A 277	56.870	26.059	122.049	1.00	45.70
ATOM	2209	NZ	LYS A 277	57.528	26.004	123.390	1.00	44.64
ATOM	2210	C	LYS A 277	55.432	21.683	121.242	1.00	30.26
ATOM	2211	O	LYS A 277	54.640	22.284	121.972	1.00	27.55
ATOM	2212	N	ALA A 278	55.057	21.078	120.115	1.00	30.15
ATOM	2213	CA	ALA A 278	53.662	21.096	119.676	1.00	30.51
ATOM	2214	CB	ALA A 278	53.496	20.270	118.406	1.00	28.96
ATOM	2215	C	ALA A 278	52.789	20.527	120.786	1.00	30.99
ATOM	2216	O	ALA A 278	51.735	21.067	121.108	1.00	30.36
ATOM	2217	N	PHE A 279	53.245	19.422	121.360	1.00	27.85
ATOM	2218	CA	PHE A 279	52.540	18.759	122.448	1.00	29.62
ATOM	2219	CB	PHE A 279	53.343	17.534	122.886	1.00	26.83
ATOM	2220	CG	PHE A 279	52.786	16.823	124.078	1.00	29.11
ATOM	2221	CD1	PHE A 279	51.556	16.176	124.015	1.00	28.86
ATOM	2222	CD2	PHE A 279	53.505	16.786	125.267	1.00	33.03
ATOM	2223	CE1	PHE A 279	51.054	15.500	125.121	1.00	37.90
ATOM	2224	CE2	PHE A 279	53.011	16.114	126.386	1.00	38.01
ATOM	2225	CZ	PHE A 279	51.783	15.469	126.313	1.00	36.33
ATOM	2226	C	PHE A 279	52.362	19.730	123.621	1.00	30.97
ATOM	2227	O	PHE A 279	51.265	19.853	124.184	1.00	26.26
ATOM	2228	N	ASN A 280	53.432	20.429	123.990	1.00	32.03
ATOM	2229	CA	ASN A 280	53.339	21.373	125.104	1.00	30.54
ATOM	2230	CB	ASN A 280	54.724	21.819	125.583	1.00	26.79
ATOM	2231	CG	ASN A 280	55.508	20.695	126.227	1.00	33.66
ATOM	2232	OD1	ASN A 280	54.958	19.886	126.971	1.00	34.47
ATOM	2233	ND2	ASN A 280	56.809	20.660	125.973	1.00	33.59
ATOM	2234	C	ASN A 280	52.493	22.587	124.781	1.00	30.46
ATOM	2235	O	ASN A 280	51.899	23.182	125.677	1.00	27.66
ATOM	2236	N	ILE A 281	52.429	22.960	123.509	1.00	27.32
ATOM	2237	CA	ILE A 281	51.620	24.107	123.128	1.00	31.07
ATOM	2238	CB	ILE A 281	51.878	24.517	121.666	1.00	35.08
ATOM	2239	CG2	ILE A 281	50.776	25.445	121.174	1.00	34.33
ATOM	2240	CG1	ILE A 281	53.253	25.185	121.562	1.00	33.53
ATOM	2241	CD1	ILE A 281	53.590	25.694	120.178	1.00	34.88
ATOM	2242	C	ILE A 281	50.141	23.798	123.329	1.00	31.22
ATOM	2243	O	ILE A 281	49.391	24.621	123.854	1.00	30.15
ATOM	2244	N	VAL A 282	49.723	22.606	122.923	1.00	30.91

ATOM	2245	CA	VAL	A	282	48.332	22.214	123.081	1.00	30.76
ATOM	2246	CB	VAL	A	282	48.075	20.797	122.523	1.00	35.10
ATOM	2247	CG1	VAL	A	282	46.641	20.358	122.841	1.00	28.72
ATOM	2248	CG2	VAL	A	282	48.313	20.781	121.018	1.00	28.66
ATOM	2249	C	VAL	A	282	47.952	22.236	124.558	1.00	31.39
ATOM	2250	O	VAL	A	282	46.884	22.715	124.917	1.00	32.70
ATOM	2251	N	ARG	A	283	48.837	21.720	125.406	1.00	29.86
ATOM	2252	CA	ARG	A	283	48.587	21.675	126.840	1.00	34.82
ATOM	2253	CB	ARG	A	283	49.629	20.785	127.519	1.00	31.44
ATOM	2254	CG-	ARG	A	283	49.551	19.334	127.061	1.00	29.49
ATOM	2255	CD	ARG	A	283	50.729	18.539	127.554	1.00	30.67
ATOM	2256	NE	ARG	A	283	50.730	18.314	128.990	1.00	30.78
ATOM	2257	CZ	ARG	A	283	51.826	18.351	129.742	1.00	35.27
ATOM	2258	NH1	ARG	A	283	53.012	18.611	129.198	1.00	36.46
ATOM	2259	NH2	ARG	A	283	51.742	18.100	131.035	1.00	35.90
ATOM	2260	C	ARG	A	283	48.561	23.065	127.473	1.00	36.06
ATOM	2261	O	ARG	A	283	47.830	23.302	128.439	1.00	35.04
ATOM	2262	N	GLU	A	284	49.350	23.985	126.928	1.00	35.70
ATOM	2263	CA	GLU	A	284	49.376	25.348	127.448	1.00	40.93
ATOM	2264	CB	GLU	A	284	50.499	26.166	126.799	1.00	44.17
ATOM	2265	CG	GLU	A	284	51.917	25.702	127.141	1.00	56.39
ATOM	2266	CD	GLU	A	284	52.989	26.495	126.401	1.00	60.69
ATOM	2267	OE1	GLU	A	284	53.012	27.738	126.542	1.00	63.13
ATOM	2268	OE2	GLU	A	284	53.810	25.880	125.680	1.00	62.79
ATOM	2269	C	GLU	A	284	48.039	26.014	127.148	1.00	39.24
ATOM	2270	O	GLU	A	284	47.525	26.783	127.954	1.00	38.52
ATOM	2271	N	VAL	A	285	47.472	25.704	125.986	1.00	33.75
ATOM	2272	CA	VAL	A	285	46.205	26.294	125.592	1.00	35.82
ATOM	2273	CB	VAL	A	285	46.039	26.291	124.062	1.00	34.14
ATOM	2274	CG1	VAL	A	285	44.654	26.811	123.693	1.00	36.43
ATOM	2275	CG2	VAL	A	285	47.114	27.153	123.419	1.00	37.26
ATOM	2276	C	VAL	A	285	44.964	25.638	126.192	1.00	38.96
ATOM	2277	O	VAL	A	285	44.043	26.336	126.611	1.00	41.83
ATOM	2278	N	PHE	A	286	44.931	24.308	126.236	1.00	37.57
ATOM	2279	CA	PHE	A	286	43.760	23.608	126.753	1.00	35.05
ATOM	2280	CB	PHE	A	286	43.159	22.723	125.657	1.00	32.53
ATOM	2281	CG	PHE	A	286	42.544	23.490	124.529	1.00	30.15
ATOM	2282	CD1	PHE	A	286	43.104	23.459	123.256	1.00	33.96
ATOM	2283	CD2	PHE	A	286	41.398	24.245	124.736	1.00	30.30
ATOM	2284	CE1	PHE	A	286	42.527	24.170	122.202	1.00	32.96
ATOM	2285	CE2	PHE	A	286	40.813	24.958	123.693	1.00	31.67
ATOM	2286	CZ	PHE	A	286	41.381	24.919	122.419	1.00	31.66
ATOM	2287	C	PHE	A	286	43.922	22.773	128.015	1.00	35.18
ATOM	2288	O	PHE	A	286	42.984	22.080	128.409	1.00	36.97
ATOM	2289	N	GLY	A	287	45.086	22.840	128.656	1.00	30.87
ATOM	2290	CA	GLY	A	287	45.297	22.056	129.862	1.00	30.06
ATOM	2291	C	GLY	A	287	45.525	20.590	129.527	1.00	34.44
ATOM	2292	O	GLY	A	287	45.914	20.264	128.403	1.00	32.54
ATOM	2293	N	GLU	A	288	45.288	19.710	130.500	1.00	28.42
ATOM	2294	CA	GLU	A	288	45.464	18.273	130.310	1.00	32.23
ATOM	2295	CB	GLU	A	288	45.613	17.576	131.663	1.00	37.02
ATOM	2296	CG	GLU	A	288	46.910	17.864	132.411	1.00	45.36
ATOM	2297	CD	GLU	A	288	48.140	17.455	131.622	1.00	45.65
ATOM	2298	OE1	GLU	A	288	48.144	16.334	131.069	1.00	46.42
ATOM	2299	OE2	GLU	A	288	49.106	18.245	131.571	1.00	50.78
ATOM	2300	C	GLU	A	288	44.309	17.623	129.546	1.00	30.98
ATOM	2301	O	GLU	A	288	43.144	17.957	129.762	1.00	28.67
ATOM	2302	N	GLY	A	289	44.641	16.694	128.657	1.00	29.66
ATOM	2303	CA	GLY	A	289	43.625	15.999	127.886	1.00	28.08
ATOM	2304	C	GLY	A	289	43.922	14.510	127.861	1.00	30.45
ATOM	2305	O	GLY	A	289	44.618	14.007	128.739	1.00	25.90
ATOM	2306	N	VAL	A	290	43.384	13.807	126.868	1.00	26.21
ATOM	2307	CA	VAL	A	290	43.612	12.373	126.718	1.00	27.31
ATOM	2308	CB	VAL	A	290	42.288	11.626	126.412	1.00	26.53
ATOM	2309	CG1	VAL	A	290	42.554	10.148	126.204	1.00	25.36
ATOM	2310	CG2	VAL	A	290	41.308	11.822	127.565	1.00	24.38

152/263 Figure 18-36

ATOM	2311	C	VAL	A	290	44.580	12.248	125.550	1.00	24.52
ATOM	2312	O	VAL	A	290	44.307	12.743	124.461	1.00	26.84
ATOM	2313	N	TYR	A	291	45.716	11.597	125.775	1.00	23.56
ATOM	2314	CA	TYR	A	291	46.729	11.478	124.732	1.00	23.74
ATOM	2315	CB	TYR	A	291	48.092	11.817	125.342	1.00	18.40
ATOM	2316	CG	TYR	A	291	48.040	13.113	126.118	1.00	21.60
ATOM	2317	CD1	TYR	A	291	48.326	13.148	127.483	1.00	23.83
ATOM	2318	CE1	TYR	A	291	48.200	14.331	128.214	1.00	24.57
ATOM	2319	CD2	TYR	A	291	47.634	14.291	125.503	1.00	18.17
ATOM	2320	CE2	TYR	A	291	47.504	15.476	126.220	1.00	26.36
ATOM	2321	CZ	TYR	A	291	47.786	15.489	127.575	1.00	27.68
ATOM	2322	OH	TYR	A	291	47.631	16.657	128.283	1.00	28.92
ATOM	2323	C	TYR	A	291	46.768	10.118	124.044	1.00	23.03
ATOM	2324	O	TYR	A	291	46.837	9.082	124.707	1.00	20.66
ATOM	2325	N	LEU	A	292	46.755	10.142	122.711	1.00	23.96
ATOM	2326	CA	LEU	A	292	46.767	8.924	121.902	1.00	20.69
ATOM	2327	CB	LEU	A	292	45.482	8.842	121.076	1.00	22.13
ATOM	2328	CG	LEU	A	292	44.162	9.063	121.814	1.00	23.78
ATOM	2329	CD1	LEU	A	292	43.001	8.959	120.826	1.00	23.09
ATOM	2330	CD2	LEU	A	292	44.008	8.050	122.930	1.00	16.01
ATOM	2331	C	LEU	A	292	47.953	8.885	120.947	1.00	22.90
ATOM	2332	O	LEU	A	292	48.527	9.923	120.617	1.00	22.31
ATOM	2333	N	GLY	A	293	48.301	7.684	120.491	1.00	18.83
ATOM	2334	CA	GLY	A	293	49.401	7.529	119.554	1.00	24.35
ATOM	2335	C	GLY	A	293	48.908	7.846	118.154	1.00	24.22
ATOM	2336	O	GLY	A	293	48.025	8.684	117.991	1.00	20.46
ATOM	2337	N	GLY	A	294	49.459	7.177	117.148	1.00	24.63
ATOM	2338	CA	GLY	A	294	49.035	7.423	115.779	1.00	22.03
ATOM	2339	C	GLY	A	294	50.024	6.869	114.769	1.00	22.90
ATOM	2340	O	GLY	A	294	50.956	6.150	115.136	1.00	24.10
ATOM	2341	N	GLY	A	295	49.825	7.203	113.499	1.00	19.85
ATOM	2342	CA	GLY	A	295	50.721	6.724	112.458	1.00	23.33
ATOM	2343	C	GLY	A	295	52.185	7.010	112.740	1.00	19.01
ATOM	2344	O	GLY	A	295	52.541	8.094	113.196	1.00	19.39
ATOM	2345	N	GLY	A	296	53.035	6.026	112.472	1.00	25.85
ATOM	2346	CA	GLY	A	296	54.468	6.162	112.690	1.00	22.65
ATOM	2347	C	GLY	A	296	55.098	4.898	112.146	1.00	25.31
ATOM	2348	O	GLY	A	296	54.778	3.798	112.609	1.00	25.86
ATOM	2349	N	TYR	A	297	56.005	5.034	111.185	1.00	22.83
ATOM	2350	CA	TYR	A	297	56.598	3.852	110.577	1.00	23.93
ATOM	2351	CB	TYR	A	297	56.137	3.780	109.125	1.00	21.59
ATOM	2352	CG	TYR	A	297	54.660	4.084	109.035	1.00	25.85
ATOM	2353	CD1	TYR	A	297	54.203	5.402	109.017	1.00	22.28
ATOM	2354	CE1	TYR	A	297	52.842	5.695	109.089	1.00	20.19
ATOM	2355	CD2	TYR	A	297	53.713	3.062	109.116	1.00	25.28
ATOM	2356	CE2	TYR	A	297	52.352	3.346	109.190	1.00	21.83
ATOM	2357	CZ	TYR	A	297	51.927	4.666	109.181	1.00	21.81
ATOM	2358	OH	TYR	A	297	50.588	4.972	109.305	1.00	19.51
ATOM	2359	C	TYR	A	297	58.104	3.694	110.674	1.00	23.78
ATOM	2360	O	TYR	A	297	58.665	2.724	110.154	1.00	22.07
ATOM	2361	N	HIS	A	298	58.765	4.641	111.326	1.00	23.71
ATOM	2362	CA	HIS	A	298	60.204	4.534	111.517	1.00	26.33
ATOM	2363	CB	HIS	A	298	60.913	5.852	111.216	1.00	28.74
ATOM	2364	CG	HIS	A	298	62.403	5.727	111.213	1.00	33.08
ATOM	2365	CD2	HIS	A	298	63.273	5.465	112.215	1.00	31.83
ATOM	2366	ND1	HIS	A	298	63.151	5.775	110.056	1.00	32.49
ATOM	2367	CE1	HIS	A	298	64.419	5.547	110.345	1.00	29.10
ATOM	2368	NE2	HIS	A	298	64.520	5.354	111.648	1.00	38.70
ATOM	2369	C	HIS	A	298	60.371	4.188	112.996	1.00	27.81
ATOM	2370	O	HIS	A	298	60.120	5.020	113.865	1.00	25.07
ATOM	2371	N	PRO	A	299	60.829	2.963	113.297	1.00	29.37
ATOM	2372	CD	PRO	A	299	61.285	1.932	112.352	1.00	26.09
ATOM	2373	CA	PRO	A	299	61.024	2.491	114.669	1.00	29.46
ATOM	2374	CB	PRO	A	299	61.675	1.118	114.465	1.00	29.03
ATOM	2375	CG	PRO	A	299	62.411	1.306	113.137	1.00	27.34
ATOM	2376	C	PRO	A	299	61.849	3.403	115.570	1.00	31.88

ATOM	2377	O	PRO	A	299	61.480	3.622	116.724	1.00	32.45
ATOM	2378	N	TYR	A	300	62.959	3.932	115.058	1.00	27.41
ATOM	2379	CA	TYR	A	300	63.803	4.801	115.878	1.00	27.34
ATOM	2380	CB	TYR	A	300	65.163	5.058	115.207	1.00	26.84
ATOM	2381	CG	TYR	A	300	65.912	3.821	114.738	1.00	29.09
ATOM	2382	CD1	TYR	A	300	65.517	2.539	115.120	1.00	30.93
ATOM	2383	CE1	TYR	A	300	66.214	1.411	114.682	1.00	30.68
ATOM	2384	CD2	TYR	A	300	67.027	3.941	113.908	1.00	29.72
ATOM	2385	CE2	TYR	A	300	67.730	2.829	113.466	1.00	30.76
ATOM	2386	CZ	TYR	A	300	67.320	1.568	113.854	1.00	33.89
ATOM	2387	OH	TYR	A	300	68.011	0.471	113.404	1.00	34.70
ATOM	2388	C	TYR	A	300	63.113	6.134	116.137	1.00	23.44
ATOM	2389	O	TYR	A	300	63.108	6.631	117.264	1.00	23.87
ATOM	2390	N	ALA	A	301	62.530	6.711	115.092	1.00	22.19
ATOM	2391	CA	ALA	A	301	61.839	7.993	115.216	1.00	26.50
ATOM	2392	CB	ALA	A	301	61.266	8.416	113.864	1.00	24.16
ATOM	2393	C	ALA	A	301	60.715	7.878	116.237	1.00	27.86
ATOM	2394	O	ALA	A	301	60.556	8.728	117.117	1.00	22.47
ATOM	2395	N	LEU	A	302	59.940	6.808	116.110	1.00	23.27
ATOM	2396	CA	LEU	A	302	58.818	6.566	116.996	1.00	26.50
ATOM	2397	CB	LEU	A	302	58.036	5.354	116.483	1.00	26.02
ATOM	2398	CG	LEU	A	302	56.866	4.798	117.291	1.00	29.73
ATOM	2399	CD1	LEU	A	302	55.983	3.938	116.394	1.00	31.01
ATOM	2400	CD2	LEU	A	302	57.394	4.001	118.465	1.00	32.99
ATOM	2401	C	LEU	A	302	59.246	6.373	118.451	1.00	27.49
ATOM	2402	O	LEU	A	302	58.648	6.946	119.358	1.00	25.22
ATOM	2403	N	ALA	A	303	60.289	5.580	118.672	1.00	27.85
ATOM	2404	CA	ALA	A	303	60.765	5.320	120.024	1.00	27.33
ATOM	2405	CB	ALA	A	303	61.854	4.269	119.990	1.00	29.17
ATOM	2406	C	ALA	A	303	61.279	6.580	120.714	1.00	26.64
ATOM	2407	O	ALA	A	303	60.944	6.849	121.875	1.00	23.18
ATOM	2408	N	ARG	A	304	62.092	7.354	120.003	1.00	27.48
ATOM	2409	CA	ARG	A	304	62.648	8.570	120.581	1.00	25.46
ATOM	2410	CB	ARG	A	304	63.773	9.136	119.704	1.00	21.31
ATOM	2411	CG	ARG	A	304	65.005	8.231	119.562	1.00	25.98
ATOM	2412	CD	ARG	A	304	66.153	9.042	118.951	1.00	27.87
ATOM	2413	NE	ARG	A	304	65.647	9.766	117.796	1.00	36.76
ATOM	2414	CZ	ARG	A	304	66.207	10.838	117.261	1.00	30.79
ATOM	2415	NH1	ARG	A	304	67.323	11.345	117.768	1.00	30.11
ATOM	2416	NH2	ARG	A	304	65.623	11.419	116.225	1.00	36.07
ATOM	2417	C	ARG	A	304	61.585	9.634	120.803	1.00	25.46
ATOM	2418	O	ARG	A	304	61.519	10.237	121.876	1.00	24.23
ATOM	2419	N	ALA	A	305	60.741	9.854	119.802	1.00	22.22
ATOM	2420	CA	ALA	A	305	59.700	10.868	119.910	1.00	26.70
ATOM	2421	CB	ALA	A	305	58.914	10.960	118.607	1.00	28.14
ATOM	2422	C	ALA	A	305	58.749	10.626	121.072	1.00	25.54
ATOM	2423	O	ALA	A	305	58.513	11.520	121.883	1.00	24.17
ATOM	2424	N	TRP	A	306	58.189	9.426	121.160	1.00	25.66
ATOM	2425	CA	TRP	A	306	57.270	9.157	122.253	1.00	28.01
ATOM	2426	CB	TRP	A	306	56.454	7.873	122.012	1.00	18.66
ATOM	2427	CG	TRP	A	306	55.382	8.052	120.973	1.00	21.80
ATOM	2428	CD2	TRP	A	306	54.709	7.019	120.240	1.00	24.88
ATOM	2429	CE2	TRP	A	306	53.725	7.646	119.442	1.00	23.98
ATOM	2430	CE3	TRP	A	306	54.839	5.623	120.181	1.00	23.26
ATOM	2431	CD1	TRP	A	306	54.795	9.228	120.599	1.00	20.24
ATOM	2432	NE1	TRP	A	306	53.799	8.995	119.681	1.00	24.18
ATOM	2433	CZ2	TRP	A	306	52.875	6.926	118.590	1.00	24.30
ATOM	2434	CZ3	TRP	A	306	53.993	4.906	119.335	1.00	23.89
ATOM	2435	CH2	TRP	A	306	53.024	5.562	118.550	1.00	24.12
ATOM	2436	C	TRP	A	306	57.969	9.113	123.605	1.00	27.93
ATOM	2437	O	TRP	A	306	57.330	9.319	124.637	1.00	28.58
ATOM	2438	N	THR	A	307	59.273	8.851	123.615	1.00	26.76
ATOM	2439	CA	THR	A	307	60.000	8.850	124.881	1.00	22.81
ATOM	2440	CB	THR	A	307	61.457	8.319	124.730	1.00	25.54
ATOM	2441	OG1	THR	A	307	61.435	6.902	124.504	1.00	22.73
ATOM	2442	CG2	THR	A	307	62.269	8.599	125.988	1.00	24.03

ATOM	2443	C	THR	A	307	60.027	10.288	125.396	1.00	26.54
ATOM	2444	O	THR	A	307	59.925	10.526	126.604	1.00	25.34
ATOM	2445	N	LEU	A	308	60.152	11.247	124.478	1.00	21.65
ATOM	2446	CA	LEU	A	308	60.172	12.657	124.862	1.00	21.41
ATOM	2447	CB	LEU	A	308	60.442	13.558	123.642	1.00	19.20
ATOM	2448	CG	LEU	A	308	61.797	13.386	122.938	1.00	21.31
ATOM	2449	CD1	LEU	A	308	61.900	14.362	121.774	1.00	21.75
ATOM	2450	CD2	LEU	A	308	62.937	13.622	123.915	1.00	19.26
ATOM	2451	C	LEU	A	308	58.811	12.981	125.479	1.00	25.18
ATOM	2452	O	LEU	A	308	58.731	13.565	126.561	1.00	21.35
ATOM	2453	N	ILE	A	309	57.743	12.567	124.806	1.00	21.74
ATOM	2454	CA	ILE	A	309	56.394	12.799	125.298	1.00	19.23
ATOM	2455	CB	ILE	A	309	55.337	12.149	124.366	1.00	19.63
ATOM	2456	CG2	ILE	A	309	53.945	12.321	124.948	1.00	19.54
ATOM	2457	CG1	ILE	A	309	55.403	12.788	122.979	1.00	20.80
ATOM	2458	CD1	ILE	A	309	55.118	14.274	122.988	1.00	20.08
ATOM	2459	C	ILE	A	309	56.228	12.222	126.701	1.00	23.97
ATOM	2460	O	ILE	A	309	55.731	12.894	127.602	1.00	21.38
ATOM	2461	N	TRP	A	310	56.652	10.977	126.888	1.00	26.45
ATOM	2462	CA	TRP	A	310	56.525	10.342	128.192	1.00	28.35
ATOM	2463	CB	TRP	A	310	56.940	8.872	128.132	1.00	23.95
ATOM	2464	CG	TRP	A	310	56.874	8.203	129.479	1.00	29.60
ATOM	2465	CD2	TRP	A	310	55.697	7.967	130.263	1.00	31.40
ATOM	2466	CE2	TRP	A	310	56.115	7.390	131.480	1.00	32.47
ATOM	2467	CE3	TRP	A	310	54.329	8.189	130.055	1.00	32.30
ATOM	2468	CD1	TRP	A	310	57.926	7.770	130.232	1.00	33.42
ATOM	2469	NE1	TRP	A	310	57.480	7.282	131.436	1.00	30.09
ATOM	2470	CZ2	TRP	A	310	55.213	7.030	132.492	1.00	29.93
ATOM	2471	CZ3	TRP	A	310	53.432	7.831	131.062	1.00	29.72
ATOM	2472	CH2	TRP	A	310	53.881	7.259	132.265	1.00	24.53
ATOM	2473	C	TRP	A	310	57.308	11.048	129.293	1.00	33.49
ATOM	2474	O	TRP	A	310	56.820	11.137	130.426	1.00	27.59
ATOM	2475	N	CYS	A	311	58.512	11.535	128.984	1.00	29.34
ATOM	2476	CA	CYS	A	311	59.305	12.247	129.994	1.00	30.06
ATOM	2477	CB	CYS	A	311	60.722	12.538	129.479	1.00	30.08
ATOM	2478	SG	CYS	A	311	61.804	11.084	129.327	1.00	33.17
ATOM	2479	C	CYS	A	311	58.612	13.560	130.397	1.00	29.25
ATOM	2480	O	CYS	A	311	58.612	13.940	131.570	1.00	28.80
ATOM	2481	N	GLU	A	312	58.021	14.247	129.425	1.00	23.13
ATOM	2482	CA	GLU	A	312	57.308	15.496	129.696	1.00	30.31
ATOM	2483	CB	GLU	A	312	56.648	16.032	128.427	1.00	28.97
ATOM	2484	CG	GLU	A	312	57.080	17.418	127.988	1.00	41.67
ATOM	2485	CD	GLU	A	312	56.905	18.465	129.059	1.00	44.21
ATOM	2486	OE1	GLU	A	312	55.813	18.534	129.658	1.00	54.15
ATOM	2487	OE2	GLU	A	312	57.860	19.233	129.290	1.00	43.90
ATOM	2488	C	GLU	A	312	56.204	15.225	130.712	1.00	28.03
ATOM	2489	O	GLU	A	312	56.120	15.869	131.751	1.00	30.64
ATOM	2490	N	LEU	A	313	55.343	14.270	130.388	1.00	31.06
ATOM	2491	CA	LEU	A	313	54.231	13.918	131.266	1.00	36.21
ATOM	2492	CB	LEU	A	313	53.337	12.873	130.604	1.00	28.83
ATOM	2493	CG	LEU	A	313	52.493	13.342	129.429	1.00	34.62
ATOM	2494	CD1	LEU	A	313	51.818	12.146	128.788	1.00	33.05
ATOM	2495	CD2	LEU	A	313	51.471	14.357	129.914	1.00	27.27
ATOM	2496	C	LEU	A	313	54.685	13.377	132.610	1.00	33.97
ATOM	2497	O	LEU	A	313	54.131	13.730	133.644	1.00	37.26
ATOM	2498	N	SER	A	314	55.688	12.508	132.577	1.00	33.72
ATOM	2499	CA	SER	A	314	56.233	11.880	133.776	1.00	33.58
ATOM	2500	CB	SER	A	314	57.183	10.743	133.388	1.00	35.88
ATOM	2501	OG	SER	A	314	56.517	9.761	132.628	1.00	45.88
ATOM	2502	C	SER	A	314	57.002	12.846	134.659	1.00	31.54
ATOM	2503	O	SER	A	314	57.339	12.513	135.788	1.00	27.69
ATOM	2504	N	GLY	A	315	57.312	14.021	134.130	1.00	35.50
ATOM	2505	CA	GLY	A	315	58.057	14.996	134.905	1.00	36.31
ATOM	2506	C	GLY	A	315	59.518	14.634	135.099	1.00	38.47
ATOM	2507	O	GLY	A	315	60.138	15.049	136.078	1.00	41.57
ATOM	2508	N	ARG	A	316	60.089	13.862	134.181	1.00	39.32

155/263

Figure 18-39

ATOM	2509	CA	ARG A 316	61.490	13.501	134.332	1.00	39.06
ATOM	2510	CB	ARG A 316	61.641	11.982	134.413	1.00	39.16
ATOM	2511	CG	ARG A 316	61.233	11.226	133.184	1.00	39.11
ATOM	2512	CD	ARG A 316	61.426	9.744	133.429	1.00	41.21
ATOM	2513	NE	ARG A 316	60.461	9.229	134.389	1.00	40.97
ATOM	2514	CZ	ARG A 316	60.524	8.021	134.926	1.00	36.40
ATOM	2515	NH1	ARG A 316	61.511	7.209	134.598	1.00	38.93
ATOM	2516	NH2	ARG A 316	59.583	7.621	135.768	1.00	30.53
ATOM	2517	C	ARG A 316	62.369	14.083	133.230	1.00	40.17
ATOM	2518	O	ARG A 316	61.910	14.325	132.111	1.00	34.27
ATOM	2519	N	GLU A 317	63.633	14.325	133.564	1.00	41.26
ATOM	2520	CA	GLU A 317	64.580	14.905	132.619	1.00	44.42
ATOM	2521	CB	GLU A 317	65.901	15.249	133.317	1.00	46.84
ATOM	2522	CG	GLU A 317	65.756	15.996	134.629	1.00	57.66
ATOM	2523	CD	GLU A 317	65.212	15.113	135.743	1.00	65.46
ATOM	2524	OE1	GLU A 317	65.871	14.101	136.073	1.00	68.38
ATOM	2525	OE2	GLU A 317	64.129	15.425	136.287	1.00	67.24
ATOM	2526	C	GLU A 317	64.873	13.962	131.462	1.00	38.45
ATOM	2527	O	GLU A 317	64.977	12.748	131.636	1.00	38.84
ATOM	2528	N	VAL A 318	65.010	14.525	130.275	1.00	37.64
ATOM	2529	CA	VAL A 318	65.315	13.720	129.108	1.00	39.13
ATOM	2530	CB	VAL A 318	64.858	14.417	127.810	1.00	42.75
ATOM	2531	CG1	VAL A 318	65.192	13.544	126.610	1.00	41.84
ATOM	2532	CG2	VAL A 318	63.364	14.701	127.867	1.00	42.38
ATOM	2533	C	VAL A 318	66.822	13.495	129.037	1.00	38.45
ATOM	2534	O	VAL A 318	67.598	14.442	128.910	1.00	36.04
ATOM	2535	N	PRO A 319	67.261	12.236	129.156	1.00	39.54
ATOM	2536	CD	PRO A 319	66.512	10.994	129.397	1.00	40.47
ATOM	2537	CA	PRO A 319	68.695	11.949	129.088	1.00	43.85
ATOM	2538	CB	PRO A 319	68.745	10.439	129.319	1.00	44.12
ATOM	2539	CG	PRO A 319	67.419	9.986	128.745	1.00	46.48
ATOM	2540	C	PRO A 319	69.228	12.353	127.718	1.00	43.55
ATOM	2541	O	PRO A 319	68.563	12.141	126.708	1.00	43.45
ATOM	2542	N	GLU A 320	70.420	12.936	127.689	1.00	42.52
ATOM	2543	CA	GLU A 320	71.026	13.380	126.440	1.00	45.19
ATOM	2544	CB	GLU A 320	72.384	14.032	126.706	1.00	43.86
ATOM	2545	CG	GLU A 320	73.121	14.412	125.434	1.00	52.62
ATOM	2546	CD	GLU A 320	74.507	14.967	125.697	1.00	52.36
ATOM	2547	OE1	GLU A 320	75.219	15.271	124.720	1.00	56.25
ATOM	2548	OE2	GLU A 320	74.883	15.101	126.875	1.00	52.25
ATOM	2549	C	GLU A 320	71.223	12.266	125.421	1.00	43.52
ATOM	2550	O	GLU A 320	70.876	12.412	124.253	1.00	41.89
ATOM	2551	N	LYS A 321	71.781	11.150	125.867	1.00	43.35
ATOM	2552	CA	LYS A 321	72.059	10.041	124.969	1.00	43.53
ATOM	2553	CB	LYS A 321	73.561	9.808	124.879	1.00	42.78
ATOM	2554	CG	LYS A 321	74.238	9.340	126.180	1.00	49.38
ATOM	2555	CD	LYS A 321	74.272	10.396	127.307	1.00	57.82
ATOM	2556	CE	LYS A 321	72.978	10.497	128.129	1.00	53.81
ATOM	2557	NZ	LYS A 321	72.660	9.245	128.883	1.00	54.17
ATOM	2558	C	LYS A 321	71.407	8.731	125.345	1.00	41.52
ATOM	2559	O	LYS A 321	70.954	8.540	126.469	1.00	41.98
ATOM	2560	N	LEU A 322	71.378	7.820	124.382	1.00	38.64
ATOM	2561	CA	LEU A 322	70.815	6.508	124.613	1.00	40.46
ATOM	2562	CB	LEU A 322	70.442	5.845	123.289	1.00	42.22
ATOM	2563	CG	LEU A 322	69.595	6.632	122.287	1.00	42.92
ATOM	2564	CD1	LEU A 322	69.204	5.737	121.125	1.00	41.13
ATOM	2565	CD2	LEU A 322	68.361	7.148	122.967	1.00	44.41
ATOM	2566	C	LEU A 322	71.918	5.702	125.268	1.00	41.36
ATOM	2567	O	LEU A 322	73.079	5.825	124.884	1.00	44.16
ATOM	2568	N	ASN A 323	71.579	4.894	126.265	1.00	39.89
ATOM	2569	CA	ASN A 323	72.594	4.067	126.895	1.00	40.96
ATOM	2570	CB	ASN A 323	72.136	3.556	128.259	1.00	43.00
ATOM	2571	CG	ASN A 323	70.787	2.886	128.202	1.00	45.59
ATOM	2572	OD1	ASN A 323	70.482	2.151	127.264	1.00	45.71
ATOM	2573	ND2	ASN A 323	69.975	3.114	129.224	1.00	48.08
ATOM	2574	C	ASN A 323	72.828	2.894	125.954	1.00	44.88

156/263

Figure 18-40

ATOM	2575	O	ASN	A	323	72.124	2.739	124.955	1.00	46.41
ATOM	2576	N	ASN	A	324	73.809	2.062	126.268	1.00	45.98
ATOM	2577	CA	ASN	A	324	74.122	0.938	125.404	1.00	49.82
ATOM	2578	CB	ASN	A	324	75.386	0.244	125.904	1.00	53.88
ATOM	2579	CG	ASN	A	324	75.960	-0.711	124.888	1.00	60.09
ATOM	2580	OD1	ASN	A	324	75.344	-1.723	124.550	1.00	66.99
ATOM	2581	ND2	ASN	A	324	77.143	-0.386	124.378	1.00	58.06
ATOM	2582	C	ASN	A	324	72.979	-0.070	125.267	1.00	47.12
ATOM	2583	O	ASN	A	324	72.784	-0.644	124.197	1.00	43.63
ATOM	2584	N	LYS	A	325	72.220	-0.276	126.339	1.00	46.39
ATOM	2585	CA	LYS	A	325	71.106	-1.221	126.318	1.00	46.76
ATOM	2586	CB	LYS	A	325	70.428	-1.328	127.695	1.00	47.65
ATOM	2587	CG	LYS	A	325	71.292	-1.837	128.858	1.00	54.21
ATOM	2588	CD	LYS	A	325	72.160	-0.750	129.526	1.00	56.87
ATOM	2589	CE	LYS	A	325	73.329	-0.289	128.671	1.00	57.45
ATOM	2590	NZ	LYS	A	325	74.091	0.816	129.307	1.00	58.32
ATOM	2591	C	LYS	A	325	70.062	-0.791	125.296	1.00	45.17
ATOM	2592	O	LYS	A	325	69.474	-1.625	124.601	1.00	42.73
ATOM	2593	N	ALA	A	326	69.832	0.514	125.213	1.00	41.43
ATOM	2594	CA	ALA	A	326	68.861	1.054	124.276	1.00	41.61
ATOM	2595	CB	ALA	A	326	68.562	2.508	124.616	1.00	42.80
ATOM	2596	C	ALA	A	326	69.365	0.940	122.838	1.00	43.80
ATOM	2597	O	ALA	A	326	68.595	0.625	121.926	1.00	45.17
ATOM	2598	N	LYS	A	327	70.658	1.191	122.637	1.00	43.46
ATOM	2599	CA	LYS	A	327	71.235	1.120	121.296	1.00	43.26
ATOM	2600	CB	LYS	A	327	72.723	1.484	121.311	1.00	44.77
ATOM	2601	CG	LYS	A	327	73.037	2.892	121.800	1.00	50.87
ATOM	2602	CD	LYS	A	327	74.544	3.168	121.747	1.00	52.74
ATOM	2603	CE	LYS	A	327	74.916	4.508	122.377	1.00	51.30
ATOM	2604	NZ	LYS	A	327	74.256	5.670	121.715	1.00	52.72
ATOM	2605	C	LYS	A	327	71.063	-0.274	120.728	1.00	41.29
ATOM	2606	O	LYS	A	327	70.625	-0.437	119.592	1.00	38.83
ATOM	2607	N	GLU	A	328	71.403	-1.278	121.526	1.00	39.95
ATOM	2608	CA	GLU	A	328	71.276	-2.660	121.090	1.00	42.40
ATOM	2609	CB	GLU	A	328	71.875	-3.605	122.135	1.00	43.05
ATOM	2610	CG	GLU	A	328	73.369	-3.432	122.295	1.00	48.81
ATOM	2611	CD	GLU	A	328	74.096	-3.529	120.963	1.00	52.11
ATOM	2612	OE1	GLU	A	328	73.972	-4.574	120.291	1.00	55.44
ATOM	2613	OE2	GLU	A	328	74.785	-2.558	120.584	1.00	51.64
ATOM	2614	C	GLU	A	328	69.825	-3.030	120.818	1.00	39.51
ATOM	2615	O	GLU	A	328	69.536	-3.842	119.939	1.00	37.35
ATOM	2616	N	LEU	A	329	68.911	-2.444	121.582	1.00	36.37
ATOM	2617	CA	LEU	A	329	67.496	-2.717	121.380	1.00	36.03
ATOM	2618	CB	LEU	A	329	66.646	-1.958	122.400	1.00	34.66
ATOM	2619	CG	LEU	A	329	65.133	-2.110	122.213	1.00	33.88
ATOM	2620	CD1	LEU	A	329	64.755	-3.572	122.351	1.00	36.21
ATOM	2621	CD2	LEU	A	329	64.391	-1.268	123.240	1.00	34.00
ATOM	2622	C	LEU	A	329	67.120	-2.268	119.971	1.00	33.64
ATOM	2623	O	LEU	A	329	66.655	-3.061	119.162	1.00	31.29
ATOM	2624	N	LEU	A	330	67.333	-0.990	119.681	1.00	33.78
ATOM	2625	CA	LEU	A	330	67.004	-0.461	118.366	1.00	36.38
ATOM	2626	CB	LEU	A	330	67.326	1.033	118.294	1.00	30.74
ATOM	2627	CG	LEU	A	330	66.514	1.958	119.205	1.00	31.51
ATOM	2628	CD1	LEU	A	330	66.857	3.404	118.894	1.00	22.11
ATOM	2629	CD2	LEU	A	330	65.028	1.728	118.978	1.00	29.69
ATOM	2630	C	LEU	A	330	67.729	-1.201	117.246	1.00	36.49
ATOM	2631	O	LEU	A	330	67.142	-1.493	116.210	1.00	35.61
ATOM	2632	N	LYS	A	331	69.005	-1.503	117.455	1.00	37.63
ATOM	2633	CA	LYS	A	331	69.786	-2.205	116.446	1.00	41.32
ATOM	2634	CB	LYS	A	331	71.256	-2.272	116.874	1.00	44.74
ATOM	2635	CG	LYS	A	331	71.954	-0.919	116.869	1.00	44.68
ATOM	2636	CD	LYS	A	331	73.350	-0.964	117.498	1.00	51.42
ATOM	2637	CE	LYS	A	331	74.315	-1.889	116.765	1.00	53.71
ATOM	2638	NZ	LYS	A	331	73.928	-3.327	116.855	1.00	56.15
ATOM	2639	C	LYS	A	331	69.258	-3.612	116.173	1.00	42.35
ATOM	2640	O	LYS	A	331	69.310	-4.086	115.042	1.00	42.68

157/263

Figure 18-41

ATOM	2641	N	SER A 332	68.734	-4.270	117.200	1.00	41.56
ATOM	2642	CA	SER A 332	68.226	-5.629	117.039	1.00	46.88
ATOM	2643	CB	SER A 332	68.045	-6.298	118.400	1.00	42.19
ATOM	2644	OG	SER A 332	66.959	-5.714	119.096	1.00	39.55
ATOM	2645	C	SER A 332	66.896	-5.687	116.297	1.00	48.58
ATOM	2646	O	SER A 332	66.393	-6.774	116.017	1.00	45.78
ATOM	2647	N	ILE A 333	66.325	-4.531	115.979	1.00	48.27
ATOM	2648	CA	ILE A 333	65.041	-4.503	115.292	1.00	51.82
ATOM	2649	CB	ILE A 333	64.378	-3.119	115.402	1.00	52.16
ATOM	2650	CG2	ILE A 333	63.038	-3.122	114.683	1.00	52.64
ATOM	2651	CG1	ILE A 333	64.163	-2.765	116.871	1.00	52.70
ATOM	2652	CD1	ILE A 333	63.550	-1.402	117.077	1.00	56.70
ATOM	2653	C	ILE A 333	65.112	-4.887	113.820	1.00	53.43
ATOM	2654	O	ILE A 333	66.118	-4.675	113.145	1.00	56.45
ATOM	2655	N	ASP A 334	64.016	-5.461	113.344	1.00	55.53
ATOM	2656	CA	ASP A 334	63.865	-5.892	111.962	1.00	59.58
ATOM	2657	CB	ASP A 334	62.845	-7.040	111.918	1.00	62.69
ATOM	2658	CG	ASP A 334	61.546	-6.712	112.664	1.00	66.23
ATOM	2659	OD1	ASP A 334	60.795	-5.814	112.227	1.00	63.25
ATOM	2660	OD2	ASP A 334	61.277	-7.354	113.704	1.00	63.45
ATOM	2661	C	ASP A 334	63.385	-4.705	111.125	1.00	60.81
ATOM	2662	O	ASP A 334	62.239	-4.673	110.681	1.00	59.47
ATOM	2663	N	PHE A 335	64.266	-3.736	110.889	1.00	60.00
ATOM	2664	CA	PHE A 335	63.864	-2.545	110.147	1.00	59.37
ATOM	2665	CB	PHE A 335	64.247	-1.298	110.952	1.00	53.38
ATOM	2666	CG	PHE A 335	63.895	-0.013	110.275	1.00	49.13
ATOM	2667	CD1	PHE A 335	62.618	0.189	109.770	1.00	44.32
ATOM	2668	CD2	PHE A 335	64.845	0.993	110.127	1.00	49.91
ATOM	2669	CE1	PHE A 335	62.288	1.373	109.122	1.00	42.74
ATOM	2670	CE2	PHE A 335	64.526	2.180	109.483	1.00	46.40
ATOM	2671	CZ	PHE A 335	63.244	2.370	108.978	1.00	42.77
ATOM	2672	C	PHE A 335	64.334	-2.399	108.696	1.00	60.85
ATOM	2673	O	PHE A 335	63.689	-2.914	107.785	1.00	66.28
ATOM	2674	N	GLU A 336	65.430	-1.671	108.493	1.00	57.40
ATOM	2675	CA	GLU A 336	66.015	-1.411	107.174	1.00	58.96
ATOM	2676	CB	GLU A 336	65.782	-2.579	106.211	1.00	62.66
ATOM	2677	CG	GLU A 336	66.417	-2.377	104.846	1.00	68.51
ATOM	2678	CD	GLU A 336	66.277	-3.590	103.943	1.00	73.21
ATOM	2679	OE1	GLU A 336	66.753	-4.678	104.333	1.00	73.30
ATOM	2680	OE2	GLU A 336	65.697	-3.457	102.843	1.00	75.74
ATOM	2681	C	GLU A 336	65.460	-0.124	106.576	1.00	55.70
ATOM	2682	O	GLU A 336	64.281	-0.023	106.253	1.00	55.28
ATOM	2683	N	GLU A 337	66.338	0.857	106.432	1.00	54.75
ATOM	2684	CA	GLU A 337	65.986	2.167	105.905	1.00	55.99
ATOM	2685	CB	GLU A 337	67.221	3.065	105.983	1.00	51.75
ATOM	2686	CG	GLU A 337	66.926	4.536	106.092	1.00	52.28
ATOM	2687	CD	GLU A 337	66.184	4.891	107.366	1.00	43.72
ATOM	2688	OE1	GLU A 337	66.705	4.640	108.474	1.00	42.21
ATOM	2689	OE2	GLU A 337	65.072	5.425	107.256	1.00	47.31
ATOM	2690	C	GLU A 337	65.485	2.064	104.460	1.00	57.56
ATOM	2691	O	GLU A 337	66.087	1.377	103.639	1.00	58.29
ATOM	2692	N	PHE A 338	64.385	2.745	104.151	1.00	60.26
ATOM	2693	CA	PHE A 338	63.814	2.710	102.805	1.00	61.69
ATOM	2694	CB	PHE A 338	62.561	3.582	102.723	1.00	60.86
ATOM	2695	CG	PHE A 338	61.845	3.493	101.401	1.00	61.92
ATOM	2696	CD1	PHE A 338	61.054	2.391	101.094	1.00	62.99
ATOM	2697	CD2	PHE A 338	61.970	4.508	100.458	1.00	62.74
ATOM	2698	CE1	PHE A 338	60.392	2.302	99.868	1.00	65.11
ATOM	2699	CE2	PHE A 338	61.315	4.428	99.228	1.00	64.62
ATOM	2700	CZ	PHE A 338	60.523	3.322	98.934	1.00	63.87
ATOM	2701	C	PHE A 338	64.818	3.208	101.773	1.00	64.33
ATOM	2702	O	PHE A 338	64.803	2.781	100.616	1.00	62.45
ATOM	2703	N	ASP A 339	65.677	4.130	102.194	1.00	64.11
ATOM	2704	CA	ASP A 339	66.689	4.684	101.310	1.00	67.42
ATOM	2705	CB	ASP A 339	66.565	6.206	101.248	1.00	67.20
ATOM	2706	CG	ASP A 339	67.647	6.838	100.402	1.00	68.03

Figure 18-42

ATOM	2707	OD1	ASP	A	339	67.796	6.432	99.229	1.00	72.20
ATOM	2708	OD2	ASP	A	339	68.346	7.740	100.904	1.00	64.15
ATOM	2709	C	ASP	A	339	68.088	4.295	101.763	1.00	68.73
ATOM	2710	O	ASP	A	339	68.511	4.628	102.869	1.00	68.17
ATOM	2711	N	ASP	A	340	68.796	3.588	100.888	1.00	71.90
ATOM	2712	CA	ASP	A	340	70.151	3.111	101.149	1.00	73.59
ATOM	2713	CB	ASP	A	340	70.778	2.601	99.848	1.00	75.47
ATOM	2714	CG	ASP	A	340	69.953	1.511	99.195	1.00	76.03
ATOM	2715	OD1	ASP	A	340	69.761	0.449	99.823	1.00	76.90
ATOM	2716	OD2	ASP	A	340	69.492	1.718	98.054	1.00	80.23
ATOM	2717	C	ASP	A	340	71.069	4.155	101.766	1.00	72.77
ATOM	2718	O	ASP	A	340	71.618	3.946	102.845	1.00	73.08
ATOM	2719	N	GLU	A	341	71.242	5.275	101.074	1.00	73.15
ATOM	2720	CA	GLU	A	341	72.112	6.341	101.557	1.00	74.56
ATOM	2721	CB	GLU	A	341	72.917	6.924	100.390	1.00	77.06
ATOM	2722	CG	GLU	A	341	73.878	8.034	100.792	1.00	82.57
ATOM	2723	CD	GLU	A	341	74.924	7.571	101.794	1.00	85.34
ATOM	2724	OE1	GLU	A	341	75.718	6.669	101.450	1.00	86.64
ATOM	2725	OE2	GLU	A	341	74.951	8.106	102.924	1.00	85.37
ATOM	2726	C	GLU	A	341	71.327	7.453	102.245	1.00	72.47
ATOM	2727	O	GLU	A	341	70.822	8.364	101.589	1.00	76.75
ATOM	2728	N	VAL	A	342	71.228	7.381	103.566	1.00	67.86
ATOM	2729	CA	VAL	A	342	70.503	8.393	104.323	1.00	64.84
ATOM	2730	CB	VAL	A	342	69.160	7.853	104.850	1.00	66.27
ATOM	2731	CG1	VAL	A	342	68.256	7.494	103.701	1.00	67.95
ATOM	2732	CG2	VAL	A	342	69.400	6.637	105.722	1.00	65.37
ATOM	2733	C	VAL	A	342	71.305	8.871	105.520	1.00	61.75
ATOM	2734	O	VAL	A	342	71.375	10.066	105.795	1.00	64.14
ATOM	2735	N	ASP	A	343	71.912	7.925	106.225	1.00	56.79
ATOM	2736	CA	ASP	A	343	72.692	8.229	107.417	1.00	54.53
ATOM	2737	CB	ASP	A	343	73.707	9.340	107.158	1.00	56.31
ATOM	2738	CG	ASP	A	343	74.531	9.660	108.388	1.00	58.81
ATOM	2739	OD1	ASP	A	343	75.298	10.644	108.357	1.00	65.36
ATOM	2740	OD2	ASP	A	343	74.420	8.918	109.387	1.00	54.29
ATOM	2741	C	ASP	A	343	71.765	8.675	108.534	1.00	50.70
ATOM	2742	O	ASP	A	343	71.442	9.859	108.651	1.00	46.00
ATOM	2743	N	ARG	A	344	71.328	7.717	109.341	1.00	46.20
ATOM	2744	CA	ARG	A	344	70.452	8.004	110.463	1.00	41.18
ATOM	2745	CB	ARG	A	344	69.121	7.268	110.299	1.00	39.81
ATOM	2746	CG	ARG	A	344	68.289	7.711	109.098	1.00	35.08
ATOM	2747	CD	ARG	A	344	68.036	9.211	109.121	1.00	28.37
ATOM	2748	NE	ARG	A	344	67.157	9.645	108.036	1.00	30.90
ATOM	2749	CZ	ARG	A	344	67.013	10.909	107.649	1.00	31.05
ATOM	2750	NH1	ARG	A	344	67.693	11.874	108.258	1.00	30.49
ATOM	2751	NH2	ARG	A	344	66.201	11.212	106.646	1.00	31.76
ATOM	2752	C	ARG	A	344	71.147	7.561	111.742	1.00	38.46
ATOM	2753	O	ARG	A	344	70.516	7.370	112.773	1.00	34.99
ATOM	2754	N	SER	A	345	72.464	7.418	111.662	1.00	33.97
ATOM	2755	CA	SER	A	345	73.261	6.981	112.795	1.00	33.68
ATOM	2756	CB	SER	A	345	74.742	6.972	112.404	1.00	39.11
ATOM	2757	OG	SER	A	345	75.163	8.260	111.990	1.00	42.80
ATOM	2758	C	SER	A	345	73.054	7.826	114.053	1.00	31.83
ATOM	2759	O	SER	A	345	73.100	7.314	115.167	1.00	24.35
ATOM	2760	N	TYR	A	346	72.819	9.119	113.877	1.00	33.10
ATOM	2761	CA	TYR	A	346	72.614	10.003	115.015	1.00	34.50
ATOM	2762	CB	TYR	A	346	72.397	11.437	114.522	1.00	35.16
ATOM	2763	CG	TYR	A	346	71.168	11.615	113.659	1.00	39.69
ATOM	2764	CD1	TYR	A	346	69.909	11.814	114.227	1.00	36.57
ATOM	2765	CE1	TYR	A	346	68.767	11.940	113.424	1.00	40.23
ATOM	2766	CD2	TYR	A	346	71.260	11.544	112.270	1.00	39.04
ATOM	2767	CE2	TYR	A	346	70.131	11.667	111.463	1.00	38.65
ATOM	2768	CZ	TYR	A	346	68.890	11.864	112.041	1.00	37.64
ATOM	2769	OH	TYR	A	346	67.776	11.982	111.234	1.00	32.48
ATOM	2770	C	TYR	A	346	71.432	9.560	115.874	1.00	37.72
ATOM	2771	O	TYR	A	346	71.396	9.829	117.074	1.00	35.48
ATCM	2772	N	MET	A	347	70.472	8.869	115.265	1.00	35.36

159/263

Figure 18-43

ATOM	2773	CA	MET A 347	69.295	8.418	116.004	1.00	36.97
ATOM	2774	CB	MET A 347	68.226	7.868	115.052	1.00	33.45
ATOM	2775	CG	MET A 347	67.853	8.809	113.921	1.00	28.09
ATOM	2776	SD	MET A 347	66.471	8.194	112.943	1.00	32.14
ATOM	2777	CE	MET A 347	67.058	6.647	112.457	1.00	39.25
ATOM	2778	C	MET A 347	69.632	7.363	117.055	1.00	34.67
ATOM	2779	O	MET A 347	68.890	7.187	118.016	1.00	33.46
ATOM	2780	N	LEU A 348	70.747	6.663	116.880	1.00	36.42
ATOM	2781	CA	LEU A 348	71.137	5.641	117.846	1.00	34.57
ATOM	2782	CB	LEU A 348	71.841	4.476	117.152	1.00	34.16
ATOM	2783	CG	LEU A 348	71.066	3.655	116.121	1.00	35.61
ATOM	2784	CD1	LEU A 348	72.010	2.660	115.469	1.00	36.58
ATOM	2785	CD2	LEU A 348	69.906	2.935	116.788	1.00	42.34
ATOM	2786	C	LEU A 348	72.075	6.232	118.885	1.00	37.10
ATOM	2787	O	LEU A 348	72.583	5.513	119.745	1.00	37.75
ATOM	2788	N	GLU A 349	72.295	7.541	118.801	1.00	38.31
ATOM	2789	CA	GLU A 349	73.192	8.231	119.726	1.00	42.86
ATOM	2790	CB	GLU A 349	74.150	9.136	118.948	1.00	47.04
ATOM	2791	CG	GLU A 349	74.942	8.426	117.867	1.00	53.27
ATOM	2792	CD	GLU A 349	75.828	7.325	118.410	1.00	58.36
ATOM	2793	OE1	GLU A 349	76.681	7.619	119.279	1.00	59.59
ATOM	2794	OE2	GLU A 349	75.669	6.166	117.963	1.00	59.17
ATOM	2795	C	GLU A 349	72.458	9.080	120.752	1.00	41.72
ATOM	2796	O	GLU A 349	72.564	8.852	121.959	1.00	42.27
ATOM	2797	N	THR A 350	71.716	10.067	120.261	1.00	37.05
ATOM	2798	CA	THR A 350	70.992	10.976	121.135	1.00	40.78
ATOM	2799	CB	THR A 350	71.468	12.418	120.900	1.00	41.69
ATOM	2800	OG1	THR A 350	71.359	12.733	119.508	1.00	43.25
ATOM	2801	CG2	THR A 350	72.918	12.575	121.325	1.00	44.11
ATOM	2802	C	THR A 350	69.474	10.911	120.968	1.00	41.47
ATOM	2803	O	THR A 350	68.968	10.608	119.884	1.00	39.72
ATOM	2804	N	LEU A 351	68.760	11.199	122.054	1.00	38.68
ATOM	2805	CA	LEU A 351	67.299	11.185	122.056	1.00	35.91
ATOM	2806	CB	LEU A 351	66.763	11.210	123.487	1.00	35.94
ATOM	2807	CG	LEU A 351	66.752	9.890	124.251	1.00	37.67
ATOM	2808	CD1	LEU A 351	66.290	10.118	125.677	1.00	40.11
ATOM	2809	CD2	LEU A 351	65.813	8.920	123.544	1.00	39.29
ATOM	2810	C	LEU A 351	66.679	12.342	121.294	1.00	37.76
ATOM	2811	O	LEU A 351	65.747	12.149	120.512	1.00	34.86
ATOM	2812	N	LYS A 352	67.192	13.544	121.525	1.00	34.79
ATOM	2813	CA	LYS A 352	66.651	14.724	120.870	1.00	38.73
ATOM	2814	CB	LYS A 352	66.676	15.911	121.835	1.00	36.48
ATOM	2815	CG	LYS A 352	66.062	15.580	123.179	1.00	42.08
ATOM	2816	CD	LYS A 352	66.202	16.701	124.196	1.00	43.22
ATOM	2817	CE	LYS A 352	65.349	17.901	123.845	1.00	49.81
ATOM	2818	NZ	LYS A 352	65.342	18.880	124.972	1.00	52.70
ATOM	2819	C	LYS A 352	67.425	15.063	119.610	1.00	38.77
ATOM	2820	O	LYS A 352	68.654	15.098	119.601	1.00	36.21
ATOM	2821	N	ASP A 353	66.697	15.293	118.530	1.00	37.69
ATOM	2822	CA	ASP A 353	67.337	15.647	117.286	1.00	39.89
ATOM	2823	CB	ASP A 353	66.532	15.075	116.110	1.00	43.53
ATOM	2824	CG	ASP A 353	65.058	15.368	116.211	1.00	47.99
ATOM	2825	OD1	ASP A 353	64.253	14.623	115.593	1.00	38.06
ATOM	2826	OD2	ASP A 353	64.706	16.352	116.898	1.00	52.94
ATOM	2827	C	ASP A 353	67.457	17.165	117.247	1.00	39.20
ATOM	2828	O	ASP A 353	66.890	17.861	118.092	1.00	35.66
ATOM	2829	N	PRO A 354	68.244	17.696	116.302	1.00	40.75
ATOM	2830	CD	PRO A 354	69.047	17.005	115.279	1.00	40.05
ATOM	2831	CA	PRO A 354	68.426	19.145	116.179	1.00	38.41
ATOM	2832	CB	PRO A 354	69.534	19.250	115.140	1.00	36.24
ATOM	2833	CG	PRO A 354	69.190	18.095	114.225	1.00	39.41
ATOM	2834	C	PRO A 354	67.144	19.780	115.689	1.00	37.28
ATOM	2835	O	PRO A 354	66.299	19.106	115.094	1.00	31.87
ATOM	2836	N	TRP A 355	66.993	21.074	115.934	1.00	37.87
ATOM	2837	CA	TRP A 355	65.804	21.757	115.472	1.00	40.04
ATOM	2838	CB	TRP A 355	65.714	23.157	116.080	1.00	42.85

160/263 Figure 18-44

ATOM	2839	CG	TRP	A	355	64.333	23.471	116.569	1.00	53.01
ATOM	2840	CD2	TRP	A	355	63.439	24.463	116.047	1.00	54.23
ATOM	2841	CE2	TRP	A	355	62.234	24.368	116.783	1.00	52.59
ATOM	2842	CE3	TRP	A	355	63.538	25.422	115.028	1.00	52.82
ATOM	2843	CD1	TRP	A	355	63.655	22.836	117.575	1.00	51.80
ATOM	2844	NE1	TRP	A	355	62.393	23.368	117.708	1.00	51.38
ATOM	2845	CZ2	TRP	A	355	61.134	25.197	116.532	1.00	51.28
ATOM	2846	CZ3	TRP	A	355	62.444	26.245	114.779	1.00	53.22
ATOM	2847	CH2	TRP	A	355	61.257	26.126	115.531	1.00	50.50
ATOM	2848	C	TRP	A	355	65.935	21.836	113.954	1.00	37.34
ATOM	2849	O	TRP	A	355	67.041	21.929	113.422	1.00	39.01
ATOM	2850	N	ARG	A	356	64.809	21.764	113.259	1.00	36.31
ATOM	2851	CA	ARG	A	356	64.797	21.820	111.802	1.00	35.22
ATOM	2852	CB	ARG	A	356	64.317	20.469	111.252	1.00	33.36
ATOM	2853	CG	ARG	A	356	65.310	19.340	111.564	1.00	34.50
ATOM	2854	CD	ARG	A	356	64.729	17.927	111.468	1.00	28.06
ATOM	2855	NE	ARG	A	356	65.745	16.956	111.870	1.00	24.79
ATOM	2856	CZ	ARG	A	356	65.499	15.703	112.236	1.00	27.56
ATOM	2857	NH1	ARG	A	356	64.253	15.237	112.259	1.00	19.09
ATOM	2858	NH2	ARG	A	356	66.502	14.918	112.604	1.00	21.34
ATOM	2859	C	ARG	A	356	63.874	22.955	111.390	1.00	33.74
ATOM	2860	O	ARG	A	356	62.746	22.732	110.950	1.00	34.68
ATOM	2861	N	GLY	A	357	64.361	24.181	111.550	1.00	35.60
ATOM	2862	CA	GLY	A	357	63.556	25.345	111.220	1.00	35.43
ATOM	2863	C	GLY	A	357	63.719	25.932	109.830	1.00	38.08
ATOM	2864	O	GLY	A	357	64.112	25.250	108.885	1.00	37.29
ATOM	2865	N	GLY	A	358	63.406	27.218	109.721	1.00	39.67
ATOM	2866	CA	GLY	A	358	63.493	27.925	108.457	1.00	36.36
ATOM	2867	C	GLY	A	358	62.398	28.966	108.499	1.00	39.45
ATOM	2868	O	GLY	A	358	61.763	29.131	109.539	1.00	37.58
ATOM	2869	N	GLU	A	359	62.163	29.662	107.391	1.00	40.89
ATOM	2870	CA	GLU	A	359	61.121	30.682	107.358	1.00	41.37
ATOM	2871	CB	GLU	A	359	61.310	31.627	106.172	1.00	44.64
ATOM	2872	CG	GLU	A	359	60.956	30.977	104.848	1.00	52.13
ATOM	2873	CD	GLU	A	359	60.833	31.973	103.708	1.00	59.14
ATOM	2874	OE1	GLU	A	359	60.448	31.551	102.593	1.00	60.47
ATOM	2875	OE2	GLU	A	359	61.119	33.173	103.923	1.00	57.77
ATOM	2876	C	GLU	A	359	59.770	30.006	107.200	1.00	38.02
ATOM	2877	O	GLU	A	359	59.689	28.828	106.850	1.00	35.29
ATOM	2878	N	VAL	A	360	58.708	30.762	107.441	1.00	36.81
ATOM	2879	CA	VAL	A	360	57.363	30.237	107.291	1.00	35.97
ATOM	2880	CB	VAL	A	360	56.401	30.789	108.368	1.00	34.90
ATOM	2881	CG1	VAL	A	360	54.999	30.251	108.133	1.00	36.53
ATOM	2882	CG2	VAL	A	360	56.888	30.393	109.755	1.00	37.06
ATOM	2883	C	VAL	A	360	56.886	30.690	105.928	1.00	36.74
ATOM	2884	O	VAL	A	360	56.661	31.881	105.712	1.00	34.90
ATOM	2885	N	ARG	A	361	56.753	29.741	105.004	1.00	35.48
ATOM	2886	CA	ARG	A	361	56.301	30.049	103.652	1.00	38.21
ATOM	2887	CB	ARG	A	361	56.152	28.776	102.815	1.00	39.76
ATOM	2888	CG	ARG	A	361	57.416	28.342	102.098	1.00	39.93
ATOM	2889	CD	ARG	A	361	57.225	26.963	101.486	1.00	38.68
ATOM	2890	NE	ARG	A	361	57.112	25.940	102.525	1.00	39.72
ATOM	2891	CZ	ARG	A	361	56.952	24.643	102.286	1.00	38.79
ATOM	2892	NH1	ARG	A	361	56.881	24.200	101.036	1.00	32.40
ATOM	2893	NH2	ARG	A	361	56.899	23.785	103.297	1.00	36.58
ATOM	2894	C	ARG	A	361	54.996	30.807	103.603	1.00	38.98
ATOM	2895	O	ARG	A	361	54.120	30.636	104.452	1.00	39.07
ATOM	2896	N	LYS	A	362	54.880	31.634	102.573	1.00	39.95
ATOM	2897	CA	LYS	A	362	53.709	32.459	102.339	1.00	42.73
ATOM	2898	CB	LYS	A	362	53.931	33.301	101.078	1.00	44.92
ATOM	2899	CG	LYS	A	362	54.995	34.390	101.219	1.00	55.45
ATOM	2900	CD	LYS	A	362	56.351	33.842	101.671	1.00	58.28
ATOM	2901	CE	LYS	A	362	56.907	32.809	100.697	1.00	57.04
ATOM	2902	NZ	LYS	A	362	58.224	32.283	101.151	1.00	58.75
ATOM	2903	C	LYS	A	362	52.434	31.634	102.200	1.00	40.51
ATOM	2904	O	LYS	A	362	51.391	31.996	102.748	1.00	36.10

161/263

Figure 18-45

ATOM	2905	N	GLU	A	363	52.506	30.527	101.469	1.00	37.79
ATOM	2906	CA	GLU	A	363	51.313	29.705	101.295	1.00	40.96
ATOM	2907	CB	GLU	A	363	51.587	28.530	100.347	1.00	43.62
ATOM	2908	CG	GLU	A	363	52.729	27.616	100.739	1.00	47.01
ATOM	2909	CD	GLU	A	363	52.995	26.547	99.683	1.00	51.65
ATOM	2910	OE1	GLU	A	363	52.080	25.737	99.409	1.00	45.63
ATOM	2911	OE2	GLU	A	363	54.116	26.526	99.125	1.00	48.44
ATOM	2912	C	GLU	A	363	50.788	29.209	102.636	1.00	37.74
ATOM	2913	O	GLU	A	363	49.582	29.113	102.834	1.00	34.79
ATOM	2914	N	VAL	A	364	51.691	28.910	103.564	1.00	33.64
ATOM	2915	CA	VAL	A	364	51.274	28.455	104.886	1.00	32.39
ATOM	2916	CB	VAL	A	364	52.484	28.048	105.749	1.00	33.99
ATOM	2917	CG1	VAL	A	364	52.018	27.676	107.160	1.00	36.90
ATOM	2918	CG2	VAL	A	364	53.198	26.867	105.109	1.00	29.56
ATOM	2919	C	VAL	A	364	50.506	29.574	105.589	1.00	34.33
ATOM	2920	O	VAL	A	364	49.454	29.336	106.188	1.00	29.80
ATOM	2921	N	LYS	A	365	51.027	30.797	105.499	1.00	38.12
ATOM	2922	CA	LYS	A	365	50.381	31.952	106.119	1.00	36.77
ATOM	2923	CB	LYS	A	365	51.255	33.204	105.969	1.00	37.98
ATOM	2924	CG	LYS	A	365	52.629	33.084	106.610	1.00	37.99
ATOM	2925	CD	LYS	A	365	53.449	34.357	106.429	1.00	35.50
ATOM	2926	CE	LYS	A	365	54.837	34.190	107.032	1.00	40.35
ATOM	2927	NZ	LYS	A	365	55.674	35.407	106.877	1.00	43.74
ATOM	2928	C	LYS	A	365	49.025	32.191	105.468	1.00	36.62
ATOM	2929	O	LYS	A	365	48.038	32.469	106.148	1.00	33.53
ATOM	2930	N	ASP	A	366	48.968	32.073	104.147	1.00	37.05
ATOM	2931	CA	ASP	A	366	47.708	32.278	103.449	1.00	37.72
ATOM	2932	CB	ASP	A	366	47.906	32.237	101.929	1.00	40.57
ATOM	2933	CG	ASP	A	366	48.833	33.334	101.427	1.00	43.98
ATOM	2934	OD1	ASP	A	366	49.078	34.304	102.176	1.00	38.51
ATOM	2935	OD2	ASP	A	366	49.297	33.235	100.269	1.00	41.96
ATOM	2936	C	ASP	A	366	46.670	31.238	103.862	1.00	39.24
ATOM	2937	O	ASP	A	366	45.497	31.562	104.029	1.00	39.04
ATOM	2938	N	THR	A	367	47.096	29.990	104.031	1.00	38.99
ATOM	2939	CA	THR	A	367	46.167	28.935	104.432	1.00	36.80
ATOM	2940	CB	THR	A	367	46.868	27.560	104.527	1.00	33.84
ATOM	2941	OG1	THR	A	367	47.332	27.167	103.232	1.00	34.92
ATOM	2942	CG2	THR	A	367	45.904	26.509	105.046	1.00	35.11
ATOM	2943	C	THR	A	367	45.532	29.257	105.786	1.00	36.58
ATOM	2944	O	THR	A	367	44.307	29.202	105.931	1.00	30.18
ATOM	2945	N	LEU	A	368	46.363	29.581	106.776	1.00	35.32
ATOM	2946	CA	LEU	A	368	45.850	29.926	108.095	1.00	35.46
ATOM	2947	CB	LEU	A	368	46.997	30.169	109.077	1.00	34.03
ATOM	2948	CG	LEU	A	368	47.545	28.925	109.794	1.00	39.04
ATOM	2949	CD1	LEU	A	368	46.449	28.358	110.688	1.00	37.35
ATOM	2950	CD2	LEU	A	368	48.014	27.871	108.797	1.00	39.52
ATOM	2951	C	LEU	A	368	44.957	31.156	107.994	1.00	38.12
ATOM	2952	O	LEU	A	368	43.968	31.277	108.719	1.00	31.70
ATOM	2953	N	GLU	A	369	45.307	32.063	107.086	1.00	40.45
ATOM	2954	CA	GLU	A	369	44.509	33.261	106.866	1.00	45.36
ATOM	2955	CB	GLU	A	369	45.128	34.126	105.765	1.00	47.38
ATOM	2956	CG	GLU	A	369	46.020	35.228	106.283	1.00	53.81
ATOM	2957	CD	GLU	A	369	45.227	36.306	106.996	1.00	59.97
ATOM	2958	OE1	GLU	A	369	45.846	37.252	107.526	1.00	60.65
ATOM	2959	OE2	GLU	A	369	43.980	36.211	107.016	1.00	63.69
ATOM	2960	C	GLU	A	369	43.100	32.865	106.466	1.00	43.23
ATOM	2961	O	GLU	A	369	42.130	33.283	107.095	1.00	44.62
ATOM	2962	N	LYS	A	370	42.983	32.057	105.417	1.00	40.34
ATOM	2963	CA	LYS	A	370	41.666	31.631	104.977	1.00	43.36
ATOM	2964	CB	LYS	A	370	41.738	30.773	103.704	1.00	44.79
ATOM	2965	CG	LYS	A	370	42.032	31.546	102.419	1.00	48.93
ATOM	2966	CD	LYS	A	370	43.503	31.514	102.019	1.00	51.41
ATOM	2967	CE	LYS	A	370	43.921	30.116	101.561	1.00	51.14
ATOM	2968	NZ	LYS	A	370	45.339	30.062	101.091	1.00	50.34
ATOM	2969	C	LYS	A	370	40.959	30.848	106.069	1.00	43.09
ATOM	2970	O	LYS	A	370	39.745	30.977	106.248	1.00	41.34

162/263

Figure 18-46

ATOM	2971	N	ALA	A	371	41.715	30.037	106.802	1.00	39.56
ATOM	2972	CA	ALA	A	371	41.120	29.238	107.861	1.00	43.57
ATOM	2973	CB	ALA	A	371	42.193	28.440	108.594	1.00	39.11
ATOM	2974	C	ALA	A	371	40.365	30.132	108.837	1.00	46.10
ATOM	2975	O	ALA	A	371	39.230	29.829	109.210	1.00	46.07
ATOM	2976	N	LYS	A	372	40.981	31.239	109.227	1.00	46.62
ATOM	2977	CA	LYS	A	372	40.391	32.178	110.192	1.00	48.18
ATOM	2978	C	LYS	A	372	39.052	32.698	109.664	1.00	51.67
ATOM	2979	O	LYS	A	372	38.294	33.318	110.432	1.00	53.21
ATOM	2980	CB	LYS	A	372	41.334	33.364	110.413	1.00	47.22
ATOM	2981	CG	LYS	A	372	42.804	32.949	110.510	1.00	20.00
ATOM	2982	CD	LYS	A	372	43.746	34.131	110.752	1.00	20.00
ATOM	2983	CE	LYS	A	372	45.216	33.715	110.849	1.00	20.00
ATOM	2984	NZ	LYS	A	372	46.121	34.850	111.081	1.00	20.00
ATOM	2985	N	ALA	A	373	38.751	32.476	108.397	1.00	57.71
ATOM	2986	CA	ALA	A	373	37.492	32.933	107.806	1.00	58.67
ATOM	2987	CB	ALA	A	373	37.758	33.632	106.480	1.00	57.19
ATOM	2988	C	ALA	A	373	36.524	31.773	107.594	1.00	59.58
ATOM	2989	O	ALA	A	373	35.432	31.797	108.205	1.00	60.89
ATOM	2990	OXT	ALA	A	373	36.870	30.853	106.822	1.00	60.10
ATOM	3014	CB	ALA	B	2	54.881	-4.431	56.836	1.00	55.77
ATOM	3015	C	ALA	B	2	53.960	-2.137	56.480	1.00	57.58
ATOM	3016	O	ALA	B	2	54.920	-1.720	57.131	1.00	56.75
ATOM	3017	N	ALA	B	2	54.263	-3.672	54.557	1.00	58.22
ATOM	3018	CA	ALA	B	2	53.914	-3.584	56.008	1.00	58.47
ATOM	3019	N	LYS	B	3	52.919	-1.376	56.151	1.00	52.79
ATOM	3020	CA	LYS	B	3	52.855	0.022	56.543	1.00	49.68
ATOM	3021	CB	LYS	B	3	51.643	0.700	55.896	1.00	53.14
ATOM	3022	CG	LYS	B	3	51.751	0.785	54.377	1.00	53.37
ATOM	3023	CD	LYS	B	3	50.685	1.681	53.786	1.00	55.40
ATOM	3024	CE	LYS	B	3	50.808	1.783	52.277	1.00	59.51
ATOM	3025	NZ	LYS	B	3	52.140	2.323	51.884	1.00	56.88
ATOM	3026	C	LYS	B	3	52.849	0.238	58.059	1.00	46.83
ATOM	3027	O	LYS	B	3	52.389	-0.607	58.830	1.00	41.63
ATOM	3028	N	VAL	B	4	53.376	1.385	58.467	1.00	41.46
ATOM	3029	CA	VAL	B	4	53.483	1.751	59.871	1.00	40.85
ATOM	3030	CB	VAL	B	4	54.893	2.288	60.163	1.00	39.55
ATOM	3031	CG1	VAL	B	4	55.070	2.541	61.648	1.00	41.23
ATOM	3032	CG2	VAL	B	4	55.916	1.306	59.652	1.00	38.96
ATOM	3033	C	VAL	B	4	52.451	2.813	60.230	1.00	38.92
ATOM	3034	O	VAL	B	4	52.472	3.916	59.691	1.00	42.80
ATOM	3035	N	LYS	B	5	51.559	2.479	61.157	1.00	34.90
ATOM	3036	CA	LYS	B	5	50.501	3.396	61.558	1.00	31.22
ATOM	3037	CB	LYS	B	5	49.133	2.796	61.215	1.00	33.76
ATOM	3038	CG	LYS	B	5	48.841	2.623	59.726	1.00	36.60
ATOM	3039	CD	LYS	B	5	48.667	3.964	59.032	1.00	41.48
ATOM	3040	CE	LYS	B	5	48.234	3.803	57.577	1.00	43.62
ATOM	3041	NZ	LYS	B	5	49.215	3.025	56.781	1.00	42.53
ATOM	3042	C	LYS	B	5	50.512	3.749	63.038	1.00	32.67
ATOM	3043	O	LYS	B	5	51.012	2.995	63.878	1.00	25.78
ATOM	3044	N	LEU	B	6	49.937	4.906	63.343	1.00	27.07
ATOM	3045	CA	LEU	B	6	49.821	5.379	64.712	1.00	31.09
ATOM	3046	CB	LEU	B	6	50.596	6.696	64.896	1.00	30.13
ATOM	3047	CG	LEU	B	6	50.691	7.340	66.285	1.00	28.09
ATOM	3048	CD1	LEU	B	6	49.333	7.827	66.728	1.00	38.87
ATOM	3049	CD2	LEU	B	6	51.248	6.338	67.282	1.00	24.87
ATOM	3050	C	LEU	B	6	48.324	5.594	64.924	1.00	29.52
ATOM	3051	O	LEU	B	6	47.669	6.287	64.149	1.00	33.36
ATOM	3052	N	ILE	B	7	47.777	4.975	65.960	1.00	28.02
ATOM	3053	CA	ILE	B	7	46.361	5.111	66.250	1.00	23.83
ATOM	3054	CB	ILE	B	7	45.736	3.761	66.670	1.00	25.11
ATOM	3055	CG2	ILE	B	7	44.309	3.974	67.127	1.00	23.59
ATOM	3056	CG1	ILE	B	7	45.690	2.794	65.477	1.00	31.00
ATOM	3057	CD1	ILE	B	7	47.021	2.406	64.906	1.00	38.60
ATOM	3058	C	ILE	B	7	46.179	6.130	67.363	1.00	26.49
ATOM	3059	O	ILE	B	7	46.766	6.005	68.430	1.00	26.68

163/263

Figure 18-47

ATOM	3060	N	GLY	B	8	45.372	7.151	67.106	1.00	29.51
ATOM	3061	CA	GLY	B	8	45.151	8.170	68.117	1.00	30.28
ATOM	3062	C	GLY	B	8	44.217	9.273	67.667	1.00	28.79
ATOM	3063	O	GLY	B	8	43.629	9.207	66.590	1.00	19.70
ATOM	3064	N	THR	B	9	44.088	10.291	68.509	1.00	26.46
ATOM	3065	CA	THR	B	9	43.234	11.438	68.238	1.00	29.37
ATOM	3066	CB	THR	B	9	41.748	11.064	68.311	1.00	32.64
ATOM	3067	OG1	THR	B	9	40.959	12.253	68.218	1.00	30.35
ATOM	3068	CG2	THR	B	9	41.431	10.383	69.637	1.00	33.42
ATOM	3069	C	THR	B	9	43.479	12.496	69.302	1.00	33.42
ATOM	3070	O	THR	B	9	43.884	12.173	70.416	1.00	30.46
ATOM	3071	N	LEU	B	10	43.228	13.754	68.961	1.00	32.05
ATOM	3072	CA	LEU	B	10	43.396	14.840	69.914	1.00	34.75
ATOM	3073	CB	LEU	B	10	43.381	16.189	69.190	1.00	38.02
ATOM	3074	CG	LEU	B	10	44.605	16.578	68.355	1.00	40.82
ATOM	3075	CD1	LEU	B	10	44.961	15.472	67.394	1.00	43.62
ATOM	3076	CD2	LEU	B	10	44.314	17.869	67.605	1.00	34.99
ATOM	3077	C	LEU	B	10	42.272	14.809	70.945	1.00	34.25
ATOM	3078	O	LEU	B	10	42.415	15.348	72.042	1.00	33.13
ATOM	3079	N	ASP	B	11	41.158	14.169	70.595	1.00	30.61
ATOM	3080	CA	ASP	B	11	40.011	14.098	71.501	1.00	33.08
ATOM	3081	CB	ASP	B	11	38.928	13.167	70.945	1.00	37.57
ATOM	3082	CG	ASP	B	11	38.372	13.643	69.621	1.00	43.14
ATOM	3083	OD1	ASP	B	11	38.013	14.834	69.525	1.00	42.22
ATOM	3084	OD2	ASP	B	11	38.281	12.825	68.681	1.00	45.58
ATOM	3085	C	ASP	B	11	40.358	13.654	72.919	1.00	32.19
ATOM	3086	O	ASP	B	11	39.688	14.053	73.875	1.00	23.44
ATOM	3087	N	TYR	B	12	41.386	12.822	73.066	1.00	28.02
ATOM	3088	CA	TYR	B	12	41.770	12.373	74.402	1.00	32.00
ATOM	3089	CB	TYR	B	12	43.011	11.476	74.363	1.00	28.67
ATOM	3090	CG	TYR	B	12	42.821	10.108	73.737	1.00	25.33
ATOM	3091	CD1	TYR	B	12	43.338	9.823	72.475	1.00	23.74
ATOM	3092	CE1	TYR	B	12	43.235	8.546	71.924	1.00	22.85
ATOM	3093	CD2	TYR	B	12	42.183	9.077	74.436	1.00	21.93
ATOM	3094	CE2	TYR	B	12	42.074	7.793	73.889	1.00	21.99
ATOM	3095	CZ	TYR	B	12	42.605	7.538	72.640	1.00	22.99
ATOM	3096	OH	TYR	B	12	42.532	6.273	72.109	1.00	18.79
ATOM	3097	C	TYR	B	12	42.054	13.567	75.319	1.00	32.74
ATOM	3098	O	TYR	B	12	41.986	13.450	76.542	1.00	23.85
ATOM	3099	N	GLY	B	13	42.374	14.710	74.720	1.00	26.96
ATOM	3100	CA	GLY	B	13	42.658	15.900	75.501	1.00	34.92
ATOM	3101	C	GLY	B	13	41.452	16.396	76.277	1.00	36.82
ATOM	3102	O	GLY	B	13	41.580	17.228	77.176	1.00	34.10
ATOM	3103	N	LYS	B	14	40.279	15.875	75.929	1.00	37.23
ATOM	3104	CA	LYS	B	14	39.031	16.247	76.584	1.00	41.77
ATOM	3105	CB	LYS	B	14	37.925	16.406	75.537	1.00	45.82
ATOM	3106	CG	LYS	B	14	38.110	17.585	74.579	1.00	51.38
ATOM	3107	CD	LYS	B	14	37.805	18.939	75.241	1.00	57.78
ATOM	3108	CE	LYS	B	14	38.752	19.285	76.388	1.00	58.82
ATOM	3109	NZ	LYS	B	14	38.387	20.568	77.070	1.00	55.06
ATOM	3110	C	LYS	B	14	38.591	15.226	77.627	1.00	39.50
ATOM	3111	O	LYS	B	14	37.546	15.385	78.252	1.00	35.54
ATOM	3112	N	TYR	B	15	39.395	14.186	77.815	1.00	40.97
ATOM	3113	CA	TYR	B	15	39.070	13.128	78.768	1.00	44.15
ATOM	3114	CB	TYR	B	15	38.863	11.827	77.990	1.00	44.42
ATOM	3115	CG	TYR	B	15	37.850	11.972	76.876	1.00	42.02
ATOM	3116	CD1	TYR	B	15	38.064	11.389	75.634	1.00	41.06
ATOM	3117	CE1	TYR	B	15	37.138	11.530	74.603	1.00	42.76
ATOM	3118	CD2	TYR	B	15	36.678	12.703	77.065	1.00	42.99
ATOM	3119	CE2	TYR	B	15	35.748	12.851	76.048	1.00	43.30
ATOM	3120	CZ	TYR	B	15	35.984	12.261	74.816	1.00	45.49
ATOM	3121	OH	TYR	B	15	35.066	12.403	73.801	1.00	45.69
ATOM	3122	C	TYR	B	15	40.151	12.944	79.838	1.00	43.48
ATOM	3123	O	TYR	B	15	40.519	11.819	80.167	1.00	41.20
ATOM	3124	N	ARG	B	16	40.647	14.052	80.381	1.00	43.01
ATOM	3125	CA	ARG	B	16	41.686	14.012	81.410	1.00	43.70

164/263

Figure 18-48

ATOM	3126	CB	ARG	B	16	42.250	15.410	81.663	1.00	49.13
ATOM	3127	CG	ARG	B	16	42.656	16.197	80.447	1.00	54.22
ATOM	3128	CD	ARG	B	16	43.858	15.624	79.751	1.00	55.13
ATOM	3129	NE	ARG	B	16	44.303	16.549	78.718	1.00	62.87
ATOM	3130	CZ	ARG	B	16	44.628	17.818	78.951	1.00	64.92
ATOM	3131	NH1	ARG	B	16	44.556	18.308	80.182	1.00	65.86
ATOM	3132	NH2	ARG	B	16	45.022	18.600	77.954	1.00	67.15
ATOM	3133	C	ARG	B	16	41.093	13.531	82.728	1.00	42.97
ATOM	3134	O	ARG	B	16	39.882	13.593	82.927	1.00	38.44
ATOM	3135	N	TYR	B	17	41.949	13.056	83.628	1.00	39.36
ATOM	3136	CA	TYR	B	17	41.494	12.637	84.945	1.00	37.67
ATOM	3137	CB	TYR	B	17	42.500	11.679	85.584	1.00	31.69
ATOM	3138	CG	TYR	B	17	42.413	10.250	85.087	1.00	28.00
ATOM	3139	CD1	TYR	B	17	42.530	9.944	83.732	1.00	22.89
ATOM	3140	CE1	TYR	B	17	42.502	8.618	83.287	1.00	21.42
ATOM	3141	CD2	TYR	B	17	42.258	9.196	85.984	1.00	24.67
ATOM	3142	CE2	TYR	B	17	42.229	7.873	85.556	1.00	24.48
ATOM	3143	CZ	TYR	B	17	42.355	7.587	84.210	1.00	27.13
ATOM	3144	OH	TYR	B	17	42.371	6.271	83.796	1.00	19.94
ATOM	3145	C	TYR	B	17	41.377	13.927	85.765	1.00	38.94
ATOM	3146	O	TYR	B	17	41.947	14.951	85.391	1.00	39.65
ATOM	3147	N	PRO	B	18	40.647	13.893	86.891	1.00	41.27
ATOM	3148	CD	PRO	B	18	39.958	12.728	87.462	1.00	43.62
ATOM	3149	CA	PRO	B	18	40.448	15.058	87.762	1.00	45.33
ATOM	3150	CB	PRO	B	18	39.648	14.473	88.928	1.00	44.09
ATOM	3151	CG	PRO	B	18	40.096	13.015	88.933	1.00	49.22
ATOM	3152	C	PRO	B	18	41.702	15.809	88.221	1.00	45.86
ATOM	3153	O	PRO	B	18	42.789	15.244	88.317	1.00	45.44
ATOM	3154	N	LYS	B	19	41.506	17.095	88.507	1.00	48.42
ATOM	3155	CA	LYS	B	19	42.535	18.040	88.952	1.00	51.03
ATOM	3156	CB	LYS	B	19	41.873	19.122	89.814	1.00	56.35
ATOM	3157	CG	LYS	B	19	40.630	18.657	90.563	1.00	65.69
ATOM	3158	CD	LYS	B	19	40.894	17.441	91.423	1.00	68.96
ATOM	3159	CE	LYS	B	19	39.602	16.882	91.999	1.00	71.85
ATOM	3160	NZ	LYS	B	19	39.825	15.603	92.731	1.00	72.79
ATOM	3161	C	LYS	B	19	43.830	17.593	89.639	1.00	48.62
ATOM	3162	O	LYS	B	19	44.912	18.009	89.235	1.00	49.04
ATOM	3163	N	ASN	B	20	43.745	16.775	90.678	1.00	43.99
ATOM	3164	CA	ASN	B	20	44.957	16.356	91.375	1.00	43.86
ATOM	3165	CB	ASN	B	20	44.740	16.440	92.890	1.00	45.92
ATOM	3166	CG	ASN	B	20	44.418	17.848	93.355	1.00	49.44
ATOM	3167	OD1	ASN	B	20	45.194	18.779	93.138	1.00	47.72
ATOM	3168	ND2	ASN	B	20	43.268	18.011	93.999	1.00	49.42
ATOM	3169	C	ASN	B	20	45.460	14.960	91.008	1.00	39.49
ATOM	3170	O	ASN	B	20	46.496	14.521	91.494	1.00	38.24
ATOM	3171	N	HIS	B	21	44.729	14.274	90.140	1.00	36.93
ATOM	3172	CA	HIS	B	21	45.091	12.923	87.723	1.00	33.57
ATOM	3173	CB	HIS	B	21	43.948	12.299	87.924	1.00	28.67
ATOM	3174	CG	HIS	B	21	44.068	10.817	88.750	1.00	32.14
ATOM	3175	CD2	HIS	B	21	44.779	10.076	87.867	1.00	26.15
ATOM	3176	ND1	HIS	B	21	43.431	9.917	89.578	1.00	29.59
ATOM	3177	CE1	HIS	B	21	43.743	8.686	89.212	1.00	23.65
ATOM	3178	NE2	HIS	B	21	44.560	8.755	88.177	1.00	29.71
ATOM	3179	C	HIS	B	21	46.348	12.928	88.852	1.00	29.06
ATOM	3180	O	HIS	B	21	46.536	13.805	88.015	1.00	24.86
ATOM	3181	N	PRO	B	22	47.225	11.937	89.035	1.00	30.50
ATOM	3182	CD	PRO	B	22	47.187	10.802	89.976	1.00	31.51
ATOM	3183	CA	PRO	B	22	48.446	11.880	88.231	1.00	29.58
ATOM	3184	CB	PRO	B	22	49.055	10.549	88.656	1.00	33.72
ATOM	3185	CG	PRO	B	22	43.658	10.489	90.124	1.00	31.07
ATOM	3186	C	PRO	B	22	48.176	11.950	86.728	1.00	28.52
ATOM	3187	O	PRO	B	22	48.989	12.474	85.972	1.00	31.85
ATOM	3188	N	LEU	B	23	47.030	11.435	86.297	1.00	24.47
ATOM	3189	CA	LEU	B	23	46.685	11.434	84.874	1.00	27.80
ATOM	3190	CB	LEU	B	23	45.933	10.141	84.513	1.00	22.18
ATOM	3191	CG	LEU	B	23	46.760	8.852	84.556	1.00	29.32

165/263

Figure 18-49

M	3192	CD1	LEU	B	23	45.868	7.628	84.402	1.00	24.94
M	3193	CD2	LEU	B	23	47.805	8.905	83.446	1.00	24.80
M	3194	C	LEU	B	23	45.891	12.638	84.367	1.00	27.95
M	3195	O	LEU	B	23	45.166	12.528	83.373	1.00	24.42
M	3196	N	LYS	B	24	46.011	13.793	85.018	1.00	31.01
M	3197	CA	LYS	B	24	45.261	14.946	84.530	1.00	29.40
M	3198	CB	LYS	B	24	44.934	15.923	85.665	1.00	33.03
M	3199	CG	LYS	B	24	45.979	16.969	85.999	1.00	33.54
M	3200	CD	LYS	B	24	47.300	16.397	86.422	1.00	39.10
M	3201	CE	LYS	B	24	48.109	17.466	87.152	1.00	45.49
M	3202	NZ	LYS	B	24	48.224	18.737	86.380	1.00	45.95
M	3203	C	LYS	B	24	46.039	15.653	83.425	1.00	30.02
M	3204	O	LYS	B	24	45.508	16.523	82.736	1.00	28.82
M	3205	N	ILE	B	25	47.298	15.262	83.246	1.00	25.93
M	3206	CA	ILE	B	25	48.139	15.858	82.212	1.00	29.48
M	3207	CB	ILE	B	25	49.641	15.528	82.409	1.00	33.61
M	3208	CG2	ILE	B	25	50.126	16.033	83.775	1.00	32.27
M	3209	CG1	ILE	B	25	49.851	14.014	82.263	1.00	28.17
M	3210	CD1	ILE	B	25	51.310	13.584	82.188	1.00	36.32
M	3211	C	ILE	B	25	47.784	15.318	80.834	1.00	30.08
M	3212	O	ILE	B	25	47.263	14.210	80.704	1.00	25.37
M	3213	N	PRO	B	26	48.064	16.101	79.783	1.00	29.19
M	3214	CD	PRO	B	26	48.650	17.448	79.770	1.00	32.47
M	3215	CA	PRO	B	26	47.782	15.673	78.413	1.00	29.52
M	3216	CB	PRO	B	26	48.103	16.921	77.593	1.00	29.84
M	3217	CG	PRO	B	26	47.930	18.046	78.599	1.00	36.40
M	3218	C	PRO	B	26	48.789	14.561	78.137	1.00	27.64
M	3219	O	PRO	B	26	49.920	14.620	78.629	1.00	23.08
M	3220	N	ARG	B	27	48.403	13.557	77.360	1.00	23.09
M	3221	CA	ARG	B	27	49.326	12.469	77.072	1.00	23.00
M	3222	CB	ARG	B	27	48.987	11.264	77.962	1.00	26.21
M	3223	CG	ARG	B	27	49.101	11.617	79.449	1.00	17.03
M	3224	CD	ARG	B	27	48.663	10.507	80.416	1.00	26.83
M	3225	NE	ARG	B	27	49.586	9.375	80.502	1.00	22.99
M	3226	CZ	ARG	B	27	49.444	8.220	79.856	1.00	25.06
M	3227	NH1	ARG	B	27	48.408	8.022	79.059	1.00	17.74
M	3228	NH2	ARG	B	27	50.336	7.253	80.027	1.00	23.38
M	3229	C	ARG	B	27	49.329	12.097	75.595	1.00	22.54
M	3230	O	ARG	B	27	50.214	12.526	74.852	1.00	21.86
M	3231	N	VAL	B	28	48.352	11.318	75.148	1.00	20.64
M	3232	CA	VAL	B	28	48.337	10.954	73.739	1.00	26.57
M	3233	CB	VAL	B	28	47.242	9.917	73.424	1.00	30.92
M	3234	CG1	VAL	B	28	47.195	9.645	71.925	1.00	27.04
M	3235	CG2	VAL	B	28	47.535	8.616	74.172	1.00	25.45
M	3236	C	VAL	B	28	48.150	12.189	72.866	1.00	28.02
M	3237	O	VAL	B	28	48.780	12.311	71.808	1.00	30.88
M	3238	N	SER	B	29	47.298	13.112	73.304	1.00	24.30
M	3239	CA	SER	B	29	47.082	14.326	72.523	1.00	29.48
M	3240	CB	SER	B	29	45.939	15.169	73.110	1.00	31.72
M	3241	CG	SER	B	29	46.218	15.614	74.424	1.00	34.55
M	3242	C	SER	B	29	48.379	15.125	72.514	1.00	30.81
M	3243	O	SER	B	29	48.680	15.820	71.545	1.00	28.85
M	3244	N	LEU	B	30	49.157	15.003	73.589	1.00	29.63
M	3245	CA	LEU	B	30	50.427	15.721	73.679	1.00	31.59
M	3246	CB	LEU	B	30	51.046	15.593	75.079	1.00	29.49
M	3247	CG	LEU	B	30	52.066	16.660	75.513	1.00	34.37
M	3248	CD1	LEU	B	30	52.937	16.083	76.610	1.00	30.15
M	3249	CD2	LEU	B	30	52.951	17.098	74.357	1.00	32.90
M	3250	C	LEU	B	30	51.371	15.085	72.672	1.00	25.90
M	3251	O	LEU	B	30	52.052	15.777	71.913	1.00	25.10
M	3252	N	LEU	B	31	51.404	13.756	72.675	1.00	22.10
M	3253	CA	LEU	B	31	52.268	13.013	71.764	1.00	25.52
M	3254	CB	LEU	B	31	51.966	11.514	71.842	1.00	26.41
M	3255	CG	LEU	B	31	53.066	10.524	71.441	1.00	28.93
M	3256	CD1	LEU	B	31	52.425	9.198	71.042	1.00	23.69
M	3257	CD2	LEU	B	31	53.873	11.049	70.300	1.00	30.41

166/263

Figure 18-50

ATOM	3258	C	LEU	B	31	52.010	13.489	70.335	1.00	25.38
ATOM	3259	O	LEU	B	31	52.940	13.851	69.614	1.00	21.03
ATOM	3260	N	LEU	B	32	50.741	13.481	69.933	1.00	21.27
ATOM	3261	CA	LEU	B	32	50.364	13.899	68.585	1.00	27.91
ATOM	3262	CB	LEU	B	32	48.841	13.798	68.408	1.00	26.60
ATOM	3263	CG	LEU	B	32	48.195	12.419	68.614	1.00	27.30
ATOM	3264	CD1	LEU	B	32	46.699	12.504	68.321	1.00	31.60
ATOM	3265	CD2	LEU	B	32	48.837	11.391	67.708	1.00	26.90
ATOM	3266	C	LEU	B	32	50.835	15.317	68.242	1.00	26.07
ATOM	3267	O	LEU	B	32	51.458	15.533	67.205	1.00	22.45
ATOM	3268	N	ARG	B	33	50.545	16.282	69.111	1.00	28.19
ATOM	3269	CA	ARG	B	33	50.962	17.660	68.865	1.00	31.77
ATOM	3270	CB	ARG	B	33	50.395	18.601	69.930	1.00	34.22
ATOM	3271	CG	ARG	B	33	48.887	18.740	69.904	1.00	40.33
ATOM	3272	CD	ARG	B	33	48.420	19.713	70.970	1.00	47.67
ATOM	3273	NE	ARG	B	33	46.977	19.931	70.924	1.00	56.24
ATOM	3274	CZ	ARG	B	33	46.330	20.505	69.912	1.00	60.10
ATOM	3275	NH1	ARG	B	33	46.997	20.929	68.845	1.00	63.11
ATOM	3276	NH2	ARG	B	33	45.011	20.652	69.965	1.00	63.81
ATOM	3277	C	ARG	B	33	52.476	17.791	68.852	1.00	30.12
ATOM	3278	O	ARG	B	33	53.028	18.580	68.097	1.00	30.20
ATOM	3279	N	PHE	B	34	53.147	17.012	69.694	1.00	30.70
ATOM	3280	CA	PHE	B	34	54.600	17.060	69.774	1.00	29.42
ATOM	3281	CB	PHE	B	34	55.096	16.176	70.920	1.00	30.46
ATOM	3282	CG	PHE	B	34	56.556	16.358	71.248	1.00	28.56
ATOM	3283	CD1	PHE	B	34	57.001	17.515	71.885	1.00	26.92
ATOM	3284	CD2	PHE	B	34	57.481	15.373	70.932	1.00	28.88
ATOM	3285	CE1	PHE	B	34	58.346	17.684	72.206	1.00	28.15
ATOM	3286	CE2	PHE	B	34	58.831	15.530	71.246	1.00	31.47
ATOM	3287	CZ	PHE	B	34	59.265	16.689	71.887	1.00	28.15
ATOM	3288	C	PHE	B	34	55.202	16.583	68.460	1.00	33.78
ATOM	3289	O	PHE	B	34	56.049	17.259	67.873	1.00	33.71
ATOM	3290	N	LYS	B	35	54.770	15.413	67.999	1.00	28.65
ATOM	3291	CA	LYS	B	35	55.294	14.880	66.753	1.00	34.33
ATOM	3292	CB	LYS	B	35	54.684	13.509	66.454	1.00	32.97
ATOM	3293	CG	LYS	B	35	55.141	12.423	67.414	1.00	34.93
ATOM	3294	CD	LYS	B	35	54.580	11.066	67.047	1.00	41.43
ATOM	3295	CE	LYS	B	35	53.070	11.004	67.205	1.00	44.04
ATOM	3296	NZ	LYS	B	35	52.335	11.984	66.345	1.00	60.09
ATOM	3297	C	LYS	B	35	55.015	15.842	65.608	1.00	35.78
ATOM	3298	O	LYS	B	35	55.869	16.061	64.752	1.00	33.39
ATOM	3299	N	ASP	B	36	53.823	16.426	65.602	1.00	32.32
ATOM	3300	CA	ASP	B	36	53.468	17.365	64.552	1.00	36.31
ATOM	3301	CB	ASP	B	36	52.015	17.800	64.698	1.00	42.56
ATOM	3302	CG	ASP	B	36	51.617	18.822	63.661	1.00	43.03
ATOM	3303	OD1	ASP	B	36	51.812	18.544	62.461	1.00	39.17
ATOM	3304	OD2	ASP	B	36	51.111	19.897	64.043	1.00	4.34
ATOM	3305	C	ASP	B	36	54.371	18.590	64.578	1.00	6.14
ATOM	3306	O	ASP	B	36	54.764	19.099	63.534	1.00	32.40
ATOM	3307	N	ALA	B	37	54.694	19.061	65.777	1.00	34.80
ATOM	3308	CA	ALA	B	37	55.554	20.226	65.924	1.00	36.82
ATOM	3309	CB	ALA	B	37	55.599	20.659	67.383	1.00	38.54
ATOM	3310	C	ALA	B	37	56.959	19.901	65.429	1.00	37.66
ATOM	3311	O	ALA	B	37	57.675	20.776	64.950	1.00	30.56
ATOM	3312	N	MET	B	38	57.346	18.635	65.541	1.00	37.42
ATOM	3313	CA	MET	B	38	58.670	18.192	65.107	1.00	36.25
ATOM	3314	CB	MET	B	38	59.158	17.059	66.013	1.00	36.44
ATOM	3315	CG	MET	B	38	59.341	17.438	67.474	1.00	37.68
ATOM	3316	SD	MET	B	38	60.841	18.391	67.784	1.00	38.07
ATOM	3317	CE	MET	B	38	62.093	17.228	67.300	1.00	30.98
ATOM	3318	C	MET	B	38	58.639	17.690	63.663	1.00	35.86
ATOM	3319	O	MET	B	38	59.659	17.262	63.130	1.00	32.69
ATOM	3320	N	ASN	B	39	57.470	17.742	63.035	1.00	35.82
ATOM	3321	CA	ASN	B	39	57.321	17.262	61.661	1.00	42.75
ATOM	3322	CB	ASN	B	39	58.156	18.108	60.688	1.00	46.20
ATOM	3323	CG	ASN	B	39	57.670	19.543	60.591	1.00	47.57

ATOM	3324	OD1	ASN	B	39	56.524	19.801	60.212	1.00	48.78
ATOM	3325	ND2	ASN	B	39	58.540	20.486	60.933	1.00	46.52
ATOM	3326	C	ASN	B	39	57.759	15.804	61.569	1.00	39.12
ATOM	3327	O	ASN	B	39	58.465	15.416	60.639	1.00	35.75
ATOM	3328	N	LEU	B	40	57.332	14.997	62.535	1.00	34.64
ATOM	3329	CA	LEU	B	40	57.700	13.590	62.556	1.00	35.10
ATOM	3330	CB	LEU	B	40	58.347	13.248	63.898	1.00	35.97
ATOM	3331	CG	LEU	B	40	59.595	14.073	64.227	1.00	36.21
ATOM	3332	CD1	LEU	B	40	60.148	13.648	65.573	1.00	36.57
ATOM	3333	CD2	LEU	B	40	60.646	13.880	63.145	1.00	36.79
ATOM	3334	C	LEU	B	40	56.549	12.626	62.264	1.00	37.58
ATOM	3335	O	LEU	B	40	56.637	11.438	62.573	1.00	39.15
ATOM	3336	N	ILE	B	41	55.476	13.131	61.663	1.00	36.79
ATOM	3337	CA	ILE	B	41	54.340	12.290	61.314	1.00	35.42
ATOM	3338	CB	ILE	B	41	53.445	11.991	62.536	1.00	35.21
ATOM	3339	CG2	ILE	B	41	52.793	13.271	63.047	1.00	31.89
ATOM	3340	CG1	ILE	B	41	52.367	10.980	62.141	1.00	32.68
ATOM	3341	CD1	ILE	B	41	51.470	10.550	63.285	1.00	36.46
ATOM	3342	C	ILE	B	41	53.492	12.937	60.229	1.00	37.52
ATOM	3343	O	ILE	B	41	53.352	14.157	60.183	1.00	40.24
ATOM	3344	N	ASP	B	42	52.943	12.114	59.345	1.00	39.55
ATOM	3345	CA	ASP	B	42	52.094	12.615	58.273	1.00	45.30
ATOM	3346	CB	ASP	B	42	52.569	12.119	56.901	1.00	45.93
ATOM	3347	CG	ASP	B	42	53.972	12.584	56.564	1.00	47.09
ATOM	3348	OD1	ASP	B	42	54.244	13.799	56.686	1.00	46.60
ATOM	3349	OD2	ASP	B	42	54.797	11.736	56.162	1.00	45.16
ATOM	3350	C	ASP	B	42	50.677	12.134	58.524	1.00	45.15
ATOM	3351	O	ASP	B	42	50.467	11.051	59.069	1.00	47.06
ATOM	3352	N	GLU	B	43	49.707	12.944	58.121	1.00	48.13
ATOM	3353	CA	GLU	B	43	48.303	12.618	58.312	1.00	50.50
ATOM	3354	CB	GLU	B	43	47.441	13.637	57.571	1.00	53.54
ATOM	3355	CG	GLU	B	43	45.961	13.505	57.840	1.00	59.52
ATOM	3356	CD	GLU	B	43	45.155	14.518	57.065	1.00	64.03
ATOM	3357	OE1	GLU	B	43	43.914	14.535	57.215	1.00	68.54
ATOM	3358	OE2	GLU	B	43	45.765	15.298	56.301	1.00	66.95
ATOM	3359	C	GLU	B	43	47.972	11.205	57.836	1.00	47.81
ATOM	3360	O	GLU	B	43	47.092	10.547	58.390	1.00	49.67
ATOM	3361	N	LYS	B	44	48.690	10.744	56.817	1.00	46.21
ATOM	3362	CA	LYS	B	44	48.484	9.409	56.251	1.00	48.28
ATOM	3363	CB	LYS	B	44	49.207	9.311	54.894	1.00	49.96
ATOM	3364	CG	LYS	B	44	49.639	7.903	54.470	1.00	52.18
ATOM	3365	CD	LYS	B	44	50.970	7.532	55.127	1.00	61.03
ATOM	3366	CE	LYS	B	44	51.399	6.095	54.844	1.00	62.80
ATOM	3367	NZ	LYS	B	44	50.511	5.098	55.510	1.00	65.34
ATOM	3368	C	LYS	B	44	48.899	8.249	57.161	1.00	45.92
ATOM	3369	O	LYS	B	44	48.418	7.127	57.009	1.00	41.30
ATOM	3370	N	GLU	B	45	49.797	8.517	58.100	1.00	42.18
ATOM	3371	CA	GLU	B	45	50.268	7.486	59.014	1.00	38.41
ATOM	3372	CB	GLU	B	45	51.684	7.812	59.468	1.00	33.73
ATOM	3373	CG	GLU	B	45	52.694	7.887	58.351	1.00	37.58
ATOM	3374	CD	GLU	B	45	53.998	8.504	58.813	1.00	34.34
ATOM	3375	OE1	GLU	B	45	53.997	9.699	59.176	1.00	38.04
ATOM	3376	OE2	GLU	B	45	55.020	7.799	58.821	1.00	33.37
ATOM	3377	C	GLU	B	45	49.368	7.403	60.238	1.00	36.86
ATOM	3378	O	GLU	B	45	49.461	6.462	61.032	1.00	34.98
ATOM	3379	N	LEU	B	46	48.489	8.386	60.386	1.00	30.86
ATOM	3380	CA	LEU	B	46	47.608	8.438	61.545	1.00	30.65
ATOM	3381	CB	LEU	B	46	47.501	9.889	62.019	1.00	32.74
ATOM	3382	CG	LEU	B	46	46.642	10.163	63.250	1.00	34.76
ATOM	3383	CD1	LEU	B	46	47.189	9.379	64.425	1.00	32.24
ATOM	3384	CD2	LEU	B	46	46.639	11.656	63.548	1.00	33.94
ATOM	3385	C	LEU	B	46	46.212	7.861	61.318	1.00	31.36
ATOM	3386	O	LEU	B	46	45.530	8.218	60.363	1.00	31.78
ATOM	3387	N	ILE	B	47	45.801	6.957	62.203	1.00	31.18
ATOM	3388	CA	ILE	B	47	44.479	6.338	62.139	1.00	29.36
ATOM	3389	CB	ILE	B	47	44.564	4.802	62.258	1.00	28.62

Figure 18-52

ATOM	3390	CG2	ILE	B	47	43.161	4.205	62.407	1.00	28.80
ATOM	3391	CG1	ILE	B	47	45.266	4.230	61.028	1.00	29.42
ATOM	3392	CD1	ILE	B	47	45.419	2.722	61.054	1.00	31.12
ATOM	3393	C	ILE	B	47	43.659	6.875	63.303	1.00	32.22
ATOM	3394	O	ILE	B	47	44.063	6.755	64.461	1.00	31.17
ATOM	3395	N	LYS	B	48	42.514	7.475	62.999	1.00	28.39
ATOM	3396	CA	LYS	B	48	41.662	8.037	64.340	1.00	32.37
ATOM	3397	CB	LYS	B	48	40.517	8.840	63.414	1.00	36.32
ATOM	3398	CG	LYS	B	48	39.607	9.514	64.430	1.00	43.08
ATOM	3399	CD	LYS	B	48	38.535	10.361	63.747	1.00	44.38
ATOM	3400	CE	LYS	B	48	37.657	11.074	64.768	1.00	45.91
ATOM	3401	NZ	LYS	B	48	38.451	11.991	65.643	1.00	42.66
ATOM	3402	C	LYS	B	48	41.095	6.943	64.937	1.00	31.08
ATOM	3403	O	LYS	B	48	40.524	5.962	64.457	1.00	26.24
ATOM	3404	N	SER	B	49	41.260	7.121	66.244	1.00	27.89
ATOM	3405	CA	SER	B	49	40.770	6.168	67.232	1.00	25.17
ATOM	3406	CB	SER	B	49	41.146	6.639	68.642	1.00	24.41
ATOM	3407	OG	SER	B	49	42.539	6.858	68.777	1.00	31.79
ATOM	3408	C	SER	B	49	39.248	6.054	67.160	1.00	29.07
ATOM	3409	O	SER	B	49	38.565	7.034	66.879	1.00	28.47
ATOM	3410	N	ARG	B	50	38.723	4.859	67.409	1.00	26.13
ATOM	3411	CA	ARG	B	50	37.278	4.658	67.430	1.00	24.24
ATOM	3412	CB	ARG	B	50	36.810	3.700	66.323	1.00	25.03
ATOM	3413	CG	ARG	B	50	37.231	2.233	66.507	1.00	26.54
ATOM	3414	CD	ARG	B	50	36.570	1.340	65.452	1.00	26.21
ATOM	3415	NE	ARG	B	50	37.006	-0.058	65.504	1.00	25.13
ATOM	3416	CZ	ARG	B	50	36.700	-0.924	66.468	1.00	26.09
ATOM	3417	NH1	ARG	B	50	35.941	-0.558	67.497	1.00	23.42
ATOM	3418	NH2	ARG	B	50	37.157	-2.168	66.402	1.00	23.91
ATOM	3419	C	ARG	B	50	36.937	4.037	68.775	1.00	23.83
ATOM	3420	O	ARG	B	50	37.782	3.392	69.403	1.00	21.60
ATOM	3421	N	PRO	B	51	35.700	4.223	69.243	1.00	22.99
ATOM	3422	CD	PRO	B	51	34.554	4.962	68.688	1.00	25.09
ATOM	3423	CA	PRO	B	51	35.338	3.628	70.530	1.00	25.48
ATOM	3424	CB	PRO	B	51	33.949	4.217	70.802	1.00	26.32
ATOM	3425	CG	PRO	B	51	33.936	5.503	69.953	1.00	28.65
ATOM	3426	C	PRO	B	51	35.264	2.118	70.325	1.00	26.73
ATOM	3427	O	PRO	B	51	35.142	1.646	69.194	1.00	18.87
ATOM	3428	N	ALA	B	52	35.355	1.359	71.408	1.00	23.64
ATOM	3429	CA	ALA	B	52	35.237	-0.083	71.291	1.00	23.27
ATOM	3430	CB	ALA	B	52	35.811	-0.757	72.521	1.00	26.31
ATOM	3431	C	ALA	B	52	33.733	-0.324	71.223	1.00	25.25
ATOM	3432	O	ALA	B	52	32.950	0.515	71.677	1.00	22.78
ATOM	3433	N	THR	B	53	33.321	-1.447	70.651	1.00	22.77
ATOM	3434	CA	THR	B	53	31.900	-1.760	70.596	1.00	26.90
ATOM	3435	CB	THR	B	53	31.567	-2.732	69.456	1.00	30.00
ATOM	3436	OG1	THR	B	53	32.305	-3.950	69.642	1.00	25.59
ATOM	3437	CG2	THR	B	53	31.917	-2.117	68.103	1.00	23.33
ATOM	3438	C	THR	B	53	31.579	-2.445	71.916	1.00	30.41
ATOM	3439	O	THR	B	53	32.484	-2.917	72.609	1.00	26.13
ATOM	3440	N	LYS	B	54	30.300	-2.504	72.268	1.00	29.12
ATOM	3441	CA	LYS	B	54	29.909	-3.140	73.514	1.00	30.24
ATOM	3442	CB	LYS	B	54	28.396	-3.027	73.720	1.00	32.78
ATOM	3443	CG	LYS	B	54	27.947	-3.351	75.131	1.00	34.85
ATOM	3444	CD	LYS	B	54	26.445	-3.204	75.268	1.00	41.13
ATOM	3445	CE	LYS	B	54	26.008	-3.366	76.709	1.00	43.39
ATOM	3446	NZ	LYS	B	54	26.464	-2.257	77.582	1.00	47.39
ATOM	3447	C	LYS	B	54	30.329	-4.603	73.442	1.00	29.10
ATOM	3448	O	LYS	B	54	30.779	-5.183	74.430	1.00	26.71
ATOM	3449	N	GLU	B	55	30.196	-5.187	72.256	1.00	23.97
ATOM	3450	CA	GLU	B	55	30.577	-6.577	72.032	1.00	28.08
ATOM	3451	CB	GLU	B	55	30.288	-6.965	70.579	1.00	24.82
ATOM	3452	CG	GLU	B	55	30.671	-8.400	70.237	1.00	33.40
ATOM	3453	CD	GLU	B	55	30.453	-8.737	68.767	1.00	38.49
ATOM	3454	OE1	GLU	B	55	30.638	-9.913	68.394	1.00	41.24
ATOM	3455	OE2	GLU	B	55	30.101	-7.833	67.984	1.00	40.02

ATOM	3456	C	GLU	B	55	32.066	-6.808	72.345	1.00	25.82
ATOM	3457	O	GLU	B	55	32.429	-7.765	73.033	1.00	23.83
ATOM	3458	N	GLU	B	56	32.931	-5.938	71.835	1.00	25.04
ATOM	3459	CA	GLU	B	56	34.365	-6.079	72.093	1.00	25.30
ATOM	3460	CB	GLU	B	56	35.141	-5.003	71.334	1.00	24.31
ATOM	3461	CG	GLU	B	56	34.866	-5.039	69.836	1.00	32.15
ATOM	3462	CD	GLU	B	56	35.512	-3.903	69.073	1.00	31.43
ATOM	3463	OE1	GLU	B	56	35.486	-2.759	69.568	1.00	28.54
ATOM	3464	OE2	GLU	B	56	36.012	-4.147	67.959	1.00	28.89
ATOM	3465	C	GLU	B	56	34.653	-5.988	73.595	1.00	28.88
ATOM	3466	O	GLU	B	56	35.450	-6.766	74.137	1.00	25.07
ATOM	3467	N	LEU	B	57	33.996	-5.050	74.272	1.00	24.52
ATOM	3468	CA	LEU	B	57	34.203	-4.891	75.702	1.00	27.34
ATOM	3469	CB	LEU	B	57	33.416	-3.694	76.231	1.00	22.79
ATOM	3470	CG	LEU	B	57	33.859	-2.320	75.722	1.00	23.57
ATOM	3471	CD1	LEU	B	57	33.008	-1.247	76.366	1.00	22.27
ATOM	3472	CD2	LEU	B	57	35.342	-2.089	76.061	1.00	17.24
ATOM	3473	C	LEU	B	57	33.785	-6.144	76.452	1.00	26.92
ATOM	3474	O	LEU	B	57	34.458	-6.568	77.396	1.00	24.06
ATOM	3475	N	LEU	B	58	32.670	-6.732	76.029	1.00	23.35
ATOM	3476	CA	LEU	B	58	32.154	-7.931	76.674	1.00	25.60
ATOM	3477	CB	LEU	B	58	30.718	-8.207	76.221	1.00	28.50
ATOM	3478	CG	LEU	B	58	29.734	-7.110	76.649	1.00	30.91
ATOM	3479	CD1	LEU	B	58	28.323	-7.468	76.212	1.00	28.93
ATOM	3480	CD2	LEU	B	58	29.794	-6.945	78.157	1.00	33.44
ATOM	3481	C	LEU	B	58	33.027	-9.153	76.446	1.00	24.59
ATOM	3482	O	LEU	B	58	32.760	-10.216	76.991	1.00	19.76
ATOM	3483	N	LEU	B	59	34.065	-9.006	75.630	1.00	23.99
ATOM	3484	CA	LEU	B	59	34.988	-10.108	75.411	1.00	25.11
ATOM	3485	CB	LEU	B	59	36.018	-9.757	74.332	1.00	21.64
ATOM	3486	CG	LEU	B	59	35.483	-9.652	72.905	1.00	24.24
ATOM	3487	CD1	LEU	B	59	36.585	-9.177	71.975	1.00	24.25
ATOM	3488	CD2	LEU	B	59	34.957	-11.014	72.468	1.00	19.91
ATOM	3489	C	LEU	B	59	35.699	-10.371	76.733	1.00	23.84
ATOM	3490	O	LEU	B	59	36.150	-11.489	76.992	1.00	19.39
ATOM	3491	N	PHE	B	60	35.793	-9.344	77.577	1.00	21.80
ATOM	3492	CA	PHE	B	60	36.462	-9.510	78.876	1.00	23.08
ATOM	3493	CB	PHE	B	60	37.809	-8.770	78.908	1.00	18.22
ATOM	3494	CG	PHE	B	60	38.544	-8.906	80.230	1.00	21.72
ATOM	3495	CD1	PHE	B	60	38.975	-10.157	80.680	1.00	19.23
ATOM	3496	CD2	PHE	B	60	38.757	-7.791	81.048	1.00	17.75
ATOM	3497	CE1	PHE	B	60	39.602	-10.301	81.927	1.00	18.80
ATOM	3498	CE2	PHE	B	60	39.384	-7.923	82.297	1.00	19.23
ATOM	3499	CZ	PHE	B	60	39.807	-9.184	82.737	1.00	16.10
ATOM	3500	C	PHE	B	60	35.648	-9.069	80.083	1.00	21.58
ATOM	3501	O	PHE	B	60	35.508	-9.822	81.040	1.00	22.21
ATOM	3502	N	HIS	B	61	35.128	-7.847	80.055	1.00	20.65
ATOM	3503	CA	HIS	B	61	34.362	-7.336	81.184	1.00	23.32
ATOM	3504	CB	HIS	B	61	34.422	-5.807	81.229	1.00	27.60
ATOM	3505	CG	HIS	B	61	35.800	-5.259	81.440	1.00	31.83
ATOM	3506	CD2	HIS	B	61	36.466	-4.940	82.575	1.00	26.86
ATOM	3507	ND1	HIS	B	61	36.669	-5.003	80.401	1.00	34.35
ATOM	3508	CE1	HIS	B	61	37.810	-4.546	80.887	1.00	34.78
ATOM	3509	NE2	HIS	B	61	37.713	-4.499	82.204	1.00	36.27
ATOM	3510	C	HIS	B	61	32.902	-7.775	81.198	1.00	28.04
ATOM	3511	O	HIS	B	61	32.349	-8.167	80.176	1.00	25.70
ATOM	3512	N	THR	B	62	32.276	-7.691	82.367	1.00	25.25
ATOM	3513	CA	THR	B	62	30.982	-8.084	82.506	1.00	25.35
ATOM	3514	CB	THR	B	62	30.578	-8.549	83.932	1.00	25.47
ATOM	3515	CG1	THR	B	62	30.783	-7.462	84.843	1.00	28.62
ATOM	3516	CG2	THR	B	62	31.482	-9.701	84.315	1.00	21.32
ATOM	3517	C	THR	B	62	29.931	-6.942	82.162	1.00	26.06
ATOM	3518	O	THR	B	62	30.287	-5.771	82.254	1.00	24.14
ATOM	3519	N	GLU	B	63	28.718	-7.305	81.759	1.00	28.01
ATOM	3520	CA	GLU	B	63	27.681	-6.349	81.389	1.00	30.77
ATOM	3521	CB	GLU	B	63	26.374	-7.094	81.114	1.00	33.97

170/263 Figure 18-54

ATOM	3522	CG	GLU	B	63	25.213	-6.210	80.667	1.00	41.12
ATOM	3523	CD	GLU	B	63	25.189	-5.987	79.168	1.00	44.47
ATOM	3524	OE1	GLU	B	63	24.361	-5.177	78.689	1.00	42.64
ATOM	3525	OE2	GLU	B	63	25.992	-6.640	78.465	1.00	45.96
ATOM	3526	C	GLU	B	63	27.436	-5.326	82.498	1.00	27.29
ATOM	3527	O	GLU	B	63	27.381	-4.118	82.252	1.00	25.13
ATOM	3528	N	ASP	B	64	27.272	-5.834	83.713	1.00	24.38
ATOM	3529	CA	ASP	B	64	27.010	-5.023	84.897	1.00	29.27
ATOM	3530	CB	ASP	B	64	26.887	-5.944	86.112	1.00	36.30
ATOM	3531	CG	ASP	B	64	28.022	-6.935	86.198	1.00	50.77
ATOM	3532	OD1	ASP	B	64	29.128	-6.540	86.630	1.00	52.71
ATOM	3533	OD2	ASP	B	64	27.812	-8.106	85.802	1.00	51.98
ATOM	3534	C	ASP	B	64	28.075	-3.967	85.143	1.00	26.49
ATOM	3535	O	ASP	B	64	27.768	-2.806	85.422	1.00	18.33
ATOM	3536	N	TYR	B	65	29.332	-4.373	85.052	1.00	22.75
ATOM	3537	CA	TYR	B	65	30.420	-3.435	85.251	1.00	19.32
ATOM	3538	CB	TYR	B	65	31.751	-4.186	85.256	1.00	16.59
ATOM	3539	CG	TYR	B	65	32.949	-3.285	85.366	1.00	19.19
ATOM	3540	CD1	TYR	B	65	33.033	-2.328	86.383	1.00	21.35
ATOM	3541	CE1	TYR	B	65	34.135	-1.489	86.489	1.00	18.32
ATOM	3542	CD2	TYR	B	65	34.004	-3.382	84.456	1.00	18.65
ATOM	3543	CE2	TYR	B	65	35.116	-2.544	84.554	1.00	21.01
ATOM	3544	CZ	TYR	B	65	35.172	-1.601	85.573	1.00	20.61
ATOM	3545	OH	TYR	B	65	36.262	-0.775	85.682	1.00	17.77
ATOM	3546	C	TYR	B	65	30.392	-2.373	84.146	1.00	22.01
ATOM	3547	O	TYR	B	65	30.399	-1.167	84.421	1.00	18.20
ATOM	3548	N	ILE	B	66	30.330	-2.815	82.894	1.00	19.49
ATOM	3549	CA	ILE	B	66	30.305	-1.870	81.786	1.00	19.68
ATOM	3550	CB	ILE	B	66	30.208	-2.592	80.432	1.00	23.31
ATOM	3551	CG2	ILE	B	66	30.200	-1.571	79.303	1.00	21.30
ATOM	3552	CG1	ILE	B	66	31.400	-3.541	80.260	1.00	27.67
ATOM	3553	CD1	ILE	B	66	32.758	-2.839	80.291	1.00	29.29
ATOM	3554	C	ILE	B	66	29.128	-0.909	81.940	1.00	26.99
ATOM	3555	O	ILE	B	66	29.294	0.309	81.848	1.00	23.36
ATOM	3556	N	ASN	B	67	27.939	-1.447	82.198	1.00	24.98
ATOM	3557	CA	ASN	B	67	26.782	-0.580	82.363	1.00	27.70
ATOM	3558	CB	ASN	B	67	25.492	-1.389	82.580	1.00	25.58
ATOM	3559	CG	ASN	B	67	25.081	-2.183	81.341	1.00	26.91
ATOM	3560	OD1	ASN	B	67	25.199	-1.701	80.220	1.00	31.48
ATOM	3561	ND2	ASN	B	67	24.572	-3.387	81.545	1.00	23.80
ATOM	3562	C	ASN	B	67	26.982	0.401	83.513	1.00	25.34
ATOM	3563	O	ASN	B	67	26.524	1.539	83.448	1.00	22.53
ATOM	3564	N	THR	B	68	27.664	-0.031	84.568	1.00	23.65
ATOM	3565	CA	THR	B	68	27.903	0.863	85.696	1.00	25.25
ATOM	3566	CB	THR	B	68	28.516	0.119	86.891	1.00	29.08
ATOM	3567	OG1	THR	B	68	27.561	-0.826	87.396	1.00	25.94
ATOM	3568	CG2	THR	B	68	28.894	1.100	88.002	1.00	22.90
ATOM	3569	C	THR	B	68	28.818	2.009	85.287	1.00	25.91
ATOM	3570	O	THR	B	68	28.576	3.156	85.661	1.00	28.47
ATOM	3571	N	LEU	B	69	29.861	1.702	84.519	1.00	25.13
ATOM	3572	CA	LEU	B	69	30.788	2.729	84.054	1.00	24.37
ATOM	3573	CB	LEU	B	69	31.915	2.122	83.201	1.00	21.32
ATOM	3574	CG	LEU	B	69	32.960	1.231	83.889	1.00	22.33
ATOM	3575	CD1	LEU	B	69	34.006	0.786	82.859	1.00	22.57
ATOM	3576	CD2	LEU	B	69	33.643	2.000	85.008	1.00	23.20
ATOM	3577	C	LEU	B	69	30.036	3.764	83.229	1.00	23.02
ATOM	3578	O	LEU	B	69	30.190	4.966	83.444	1.00	18.98
ATOM	3579	N	MET	B	70	29.218	3.290	82.294	1.00	19.62
ATOM	3580	CA	MET	B	70	28.449	4.181	81.434	1.00	25.87
ATOM	3581	CB	MET	B	70	27.660	3.371	80.401	1.00	24.80
ATOM	3582	CG	MET	B	70	28.531	2.511	79.490	1.00	30.37
ATOM	3583	SD	MET	B	70	27.592	1.599	78.227	1.00	30.35
ATOM	3584	CE	MET	B	70	26.922	2.986	77.245	1.00	30.20
ATOM	3585	C	MET	B	70	27.489	5.062	82.242	1.00	28.82
ATOM	3586	O	MET	B	70	27.391	6.273	82.009	1.00	24.09
ATOM	3587	N	GLU	B	71	26.786	4.458	83.194	1.00	28.21

171/263

Figure 18-55

ATOM	3588	CA	GLU	B	71	25.837	5.207	84.008	1.00	27.45
ATOM	3589	CB	GLU	B	71	25.014	4.268	84.889	1.00	30.70
ATOM	3590	CG	GLU	B	71	24.072	5.005	85.832	1.00	33.61
ATOM	3591	CD	GLU	B	71	23.044	5.867	85.096	1.00	37.51
ATOM	3592	OE1	GLU	B	71	22.333	6.638	85.773	1.00	35.47
ATOM	3593	OE2	GLU	B	71	22.934	5.769	83.849	1.00	31.03
ATOM	3594	C	GLU	B	71	26.559	6.209	84.887	1.00	29.15
ATOM	3595	O	GLU	B	71	26.115	7.341	85.035	1.00	23.96
ATOM	3596	N	ALA	B	72	27.671	5.781	85.481	1.00	27.76
ATOM	3597	CA	ALA	B	72	28.454	6.662	86.340	1.00	27.58
ATOM	3598	CB	ALA	B	72	29.663	5.920	86.909	1.00	23.24
ATOM	3599	C	ALA	B	72	28.924	7.886	85.563	1.00	28.07
ATOM	3600	O	ALA	B	72	28.895	8.999	86.079	1.00	23.22
ATOM	3601	N	GLU	B	73	29.356	7.684	84.322	1.00	26.40
ATOM	3602	CA	GLU	B	73	29.846	8.801	83.529	1.00	29.06
ATOM	3603	CB	GLU	B	73	30.658	8.314	82.325	1.00	29.48
ATOM	3604	CG	GLU	B	73	31.162	9.466	81.443	1.00	31.00
ATOM	3605	CD	GLU	B	73	31.938	9.009	80.216	1.00	34.37
ATOM	3606	OE1	GLU	B	73	33.059	8.461	80.356	1.00	28.41
ATOM	3607	OE2	GLU	B	73	31.419	9.203	79.100	1.00	30.59
ATOM	3608	C	GLU	B	73	28.744	9.734	83.045	1.00	31.92
ATOM	3609	O	GLU	B	73	28.894	10.951	83.104	1.00	35.69
ATOM	3610	N	ARG	B	74	27.633	9.186	82.570	1.00	33.53
ATOM	3611	CA	ARG	B	74	26.583	10.067	82.081	1.00	38.64
ATOM	3612	CB	ARG	B	74	25.456	9.280	81.403	1.00	39.90
ATOM	3613	CG	ARG	B	74	24.448	8.706	82.363	1.00	46.67
ATOM	3614	CD	ARG	B	74	23.174	8.311	81.646	1.00	47.53
ATOM	3615	NE	ARG	B	74	22.076	8.153	82.594	1.00	55.58
ATOM	3616	CZ	ARG	B	74	21.609	9.136	83.362	1.00	56.04
ATOM	3617	NH1	ARG	B	74	22.142	10.351	83.297	1.00	58.93
ATOM	3618	NH2	ARG	B	74	20.601	8.910	84.192	1.00	53.62
ATOM	3619	C	ARG	B	74	26.008	10.914	83.222	1.00	35.84
ATOM	3620	O	ARG	B	74	25.778	12.107	83.048	1.00	29.44
ATOM	3621	N	SER	B	75	25.794	10.302	84.386	1.00	31.02
ATOM	3622	CA	SER	B	75	25.243	11.014	85.539	1.00	31.99
ATOM	3623	CB	SER	B	75	24.592	10.038	86.510	1.00	34.47
ATOM	3624	OG	SER	B	75	25.581	9.228	87.123	1.00	34.33
ATOM	3625	C	SER	B	75	26.339	11.754	86.288	1.00	35.42
ATOM	3626	O	SER	B	75	26.060	12.555	87.180	1.00	33.45
ATOM	3627	N	GLN	B	76	27.584	11.473	85.922	1.00	33.25
ATOM	3628	CA	GLN	B	76	28.739	12.082	86.565	1.00	35.61
ATOM	3629	CB	GLN	B	76	28.818	13.572	86.241	1.00	30.11
ATOM	3630	CG	GLN	B	76	30.216	14.112	86.390	1.00	39.13
ATOM	3631	CD	GLN	B	76	31.124	13.681	85.248	1.00	33.54
ATOM	3632	OE1	GLN	B	76	31.052	12.546	84.761	1.00	29.21
ATOM	3633	NE2	GLN	B	76	31.995	14.583	84.827	1.00	40.93
ATOM	3634	C	GLN	B	76	28.624	11.892	88.079	1.00	37.88
ATOM	3635	O	GLN	B	76	28.901	12.908	88.858	1.00	32.74
ATOM	3636	N	SER	B	77	28.209	10.697	88.488	1.00	34.72
ATOM	3637	CA	SER	B	77	28.047	10.382	89.901	1.00	37.07
ATOM	3638	CB	SER	B	77	26.635	10.738	90.371	1.00	39.61
ATOM	3639	CG	SER	B	77	25.678	9.941	89.688	1.00	39.03
ATOM	3640	C	SER	B	77	28.265	8.897	90.112	1.00	35.95
ATOM	3641	O	SER	B	77	28.177	8.108	89.173	1.00	36.60
ATOM	3642	N	VAL	B	78	28.528	8.518	91.355	1.00	33.03
ATOM	3643	CA	VAL	B	78	28.753	7.124	91.685	1.00	33.41
ATOM	3644	CB	VAL	B	78	29.742	6.979	92.848	1.00	36.91
ATOM	3645	CG1	VAL	B	78	29.955	5.499	93.163	1.00	34.37
ATOM	3646	CG2	VAL	B	78	31.055	7.658	92.496	1.00	34.19
ATOM	3647	C	VAL	B	78	27.461	6.431	92.082	1.00	34.93
ATOM	3648	O	VAL	B	78	26.897	6.703	93.143	1.00	28.25
ATOM	3649	N	PRO	B	79	26.971	5.521	91.228	1.00	36.73
ATOM	3650	CD	PRO	B	79	27.532	5.114	89.930	1.00	37.44
ATOM	3651	CA	PRO	B	79	25.738	4.779	91.493	1.00	38.33
ATOM	3652	CB	PRO	B	79	25.668	3.826	90.301	1.00	38.68
ATOM	3653	CG	PRO	B	79	26.293	4.664	89.201	1.00	37.41

ATOM	3654	C	PRO	B	79	25.788	4.046	92.834	1.00	36.92
ATOM	3655	O	PRO	B	79	26.854	3.648	93.298	1.00	33.03
ATOM	3656	N	LYS	B	80	24.623	3.881	93.448	1.00	38.43
ATOM	3657	CA	LYS	B	80	24.482	3.206	94.736	1.00	39.73
ATOM	3658	CB	LYS	B	80	23.003	2.871	94.967	1.00	43.33
ATOM	3659	CG	LYS	B	80	22.679	2.129	96.262	1.00	44.60
ATOM	3660	CD	LYS	B	80	21.198	1.742	96.287	1.00	48.09
ATOM	3661	CE	LYS	B	80	20.805	1.014	97.559	1.00	50.12
ATOM	3662	NZ	LYS	B	80	20.932	1.890	98.760	1.00	53.16
ATOM	3663	C	LYS	B	80	25.315	1.928	94.854	1.00	40.35
ATOM	3664	O	LYS	B	80	25.181	1.011	94.047	1.00	36.67
ATOM	3665	N	GLY	B	81	26.173	1.880	95.869	1.00	38.26
ATOM	3666	CA	GLY	B	81	26.996	0.709	96.104	1.00	34.69
ATOM	3667	C	GLY	B	81	28.066	0.407	95.071	1.00	34.63
ATOM	3668	O	GLY	B	81	28.861	-0.513	95.255	1.00	33.92
ATOM	3669	N	ALA	B	82	28.100	1.178	93.992	1.00	31.26
ATOM	3670	CA	ALA	B	82	29.082	0.963	92.936	1.00	34.88
ATOM	3671	CB	ALA	B	82	28.755	1.848	91.751	1.00	23.13
ATOM	3672	C	ALA	B	82	30.517	1.223	93.405	1.00	36.85
ATOM	3673	O	ALA	B	82	31.461	0.580	92.945	1.00	32.17
ATOM	3674	N	ARG	B	83	30.677	2.168	94.323	1.00	36.52
ATOM	3675	CA	ARG	B	83	31.994	2.522	94.830	1.00	38.75
ATOM	3676	CB	ARG	B	83	31.865	3.616	95.685	1.00	40.24
ATOM	3677	CG	ARG	B	83	33.187	4.180	96.330	1.00	49.12
ATOM	3678	CD	ARG	B	83	33.015	5.239	97.404	1.00	53.26
ATOM	3679	NE	ARG	B	83	34.240	6.010	97.624	1.00	59.30
ATOM	3680	CZ	ARG	B	83	35.437	5.486	97.883	1.00	61.56
ATOM	3681	NH1	ARG	B	83	35.598	4.170	97.958	1.00	63.53
ATOM	3682	NH2	ARG	B	83	36.479	6.285	98.073	1.00	62.02
ATOM	3683	C	ARG	B	83	32.719	1.326	95.426	1.00	37.75
ATOM	3684	O	ARG	B	83	33.893	1.094	95.146	1.00	37.18
ATOM	3685	N	GLU	B	84	32.011	0.564	96.249	1.00	35.29
ATOM	3686	CA	GLU	B	84	32.581	-0.609	96.898	1.00	35.29
ATOM	3687	CB	GLU	B	84	31.876	-0.855	98.236	1.00	40.14
ATOM	3688	CG	GLU	B	84	30.443	-0.383	98.240	1.00	46.30
ATOM	3689	CD	GLU	B	84	30.356	1.132	98.293	1.00	48.30
ATOM	3690	OE1	GLU	B	84	29.339	1.690	97.834	1.00	43.07
ATOM	3691	OE2	GLU	B	84	31.306	1.762	98.814	1.00	50.07
ATOM	3692	C	GLU	B	84	32.527	-1.880	96.055	1.00	32.90
ATOM	3693	O	GLU	B	84	33.371	-2.765	96.193	1.00	28.68
ATOM	3694	N	LYS	B	85	31.533	-1.984	95.187	1.00	27.12
ATOM	3695	CA	LYS	B	85	31.412	-3.177	94.361	1.00	30.46
ATOM	3696	CB	LYS	B	85	29.950	-3.401	93.967	1.00	30.01
ATOM	3697	CG	LYS	B	85	29.717	-4.643	93.117	1.00	28.40
ATOM	3698	CD	LYS	B	85	28.234	-4.807	92.775	1.00	32.87
ATOM	3699	CE	LYS	B	85	28.000	-6.048	91.928	1.00	34.15
ATOM	3700	NZ	LYS	B	85	26.582	-6.186	91.507	1.00	35.34
ATOM	3701	C	LYS	B	85	32.267	-3.096	93.101	1.00	28.98
ATOM	3702	O	LYS	B	85	32.817	-4.098	92.652	1.00	24.69
ATOM	3703	N	TYR	B	86	32.391	-1.896	92.550	1.00	27.81
ATOM	3704	CA	TYR	B	86	33.141	-1.692	91.319	1.00	27.56
ATOM	3705	CB	TYR	B	86	32.206	-1.050	90.288	1.00	28.88
ATOM	3706	CG	TYR	B	86	31.008	-1.927	89.951	1.00	31.29
ATOM	3707	CD1	TYR	B	86	31.178	-3.137	89.276	1.00	26.99
ATOM	3708	CE1	TYR	B	86	30.095	-3.955	88.965	1.00	26.97
ATOM	3709	CD2	TYR	B	86	29.713	-1.553	90.315	1.00	28.38
ATOM	3710	CE2	TYR	B	86	28.611	-2.370	90.008	1.00	24.19
ATOM	3711	CZ	TYR	B	86	28.815	-3.569	89.331	1.00	28.46
ATOM	3712	OH	TYR	B	86	27.747	-4.379	89.008	1.00	22.70
ATOM	3713	C	TYR	B	86	34.422	-0.870	91.489	1.00	24.64
ATOM	3714	O	TYR	B	86	35.160	-0.645	90.530	1.00	27.19
ATOM	3715	N	ASN	B	87	34.674	-0.418	92.711	1.00	25.54
ATOM	3716	CA	ASN	B	87	35.881	0.341	93.032	1.00	29.30
ATOM	3717	CB	ASN	B	87	37.105	-0.561	92.866	1.00	28.92
ATOM	3718	CG	ASN	B	87	38.343	0.019	93.506	1.00	34.72
ATOM	3719	OD1	ASN	B	87	38.309	0.452	94.659	1.00	38.41

ATOM	3720	ND2	ASN	B	87	39.449	0.012	92.775	1.00	35.86
ATOM	3721	C	ASN	B	87	36.070	1.622	92.223	1.00	29.72
ATOM	3722	O	ASN	B	87	37.194	1.998	91.876	1.00	24.01
ATOM	3723	N	ILE	B	88	34.956	2.282	91.932	1.00	29.43
ATOM	3724	CA	ILE	B	88	34.945	3.536	91.196	1.00	30.64
ATOM	3725	CB	ILE	B	88	33.959	3.464	90.027	1.00	37.12
ATOM	3726	CG2	ILE	B	88	33.821	4.829	89.379	1.00	40.62
ATOM	3727	CG1	ILE	B	88	34.421	2.433	89.008	1.00	35.43
ATOM	3728	CD1	ILE	B	88	35.684	2.821	88.324	1.00	41.80
ATOM	3729	C	ILE	B	88	34.483	4.669	92.118	1.00	31.90
ATOM	3730	O	ILE	B	88	33.681	4.445	93.024	1.00	28.86
ATOM	3731	N	GLY	B	89	34.977	5.881	91.875	1.00	30.36
ATOM	3732	CA	GLY	B	89	34.574	7.022	92.686	1.00	29.54
ATOM	3733	C	GLY	B	89	35.601	7.524	93.685	1.00	31.49
ATOM	3734	O	GLY	B	89	35.497	8.652	94.177	1.00	37.26
ATOM	3735	N	GLY	B	90	36.583	6.687	94.005	1.00	30.97
ATOM	3736	CA	GLY	B	90	37.612	7.086	94.949	1.00	31.03
ATOM	3737	C	GLY	B	90	38.655	7.936	94.247	1.00	34.78
ATOM	3738	O	GLY	B	90	38.455	8.344	93.103	1.00	32.73
ATOM	3739	N	TYR	B	91	39.772	8.201	94.915	1.00	29.39
ATOM	3740	CA	TYR	B	91	40.820	9.023	94.322	1.00	28.15
ATOM	3741	CB	TYR	B	91	41.810	9.463	95.405	1.00	27.29
ATOM	3742	CG	TYR	B	91	42.609	8.330	96.007	1.00	26.60
ATOM	3743	CD1	TYR	B	91	43.738	7.823	95.359	1.00	28.55
ATOM	3744	CE1	TYR	B	91	44.456	6.762	95.896	1.00	28.75
ATOM	3745	CD2	TYR	B	91	42.219	7.741	97.208	1.00	28.35
ATOM	3746	CE2	TYR	B	91	42.927	6.680	97.751	1.00	27.58
ATOM	3747	CZ	TYR	B	91	44.043	6.196	97.094	1.00	30.12
ATOM	3748	OH	TYR	B	91	44.753	5.154	97.637	1.00	36.59
ATOM	3749	C	TYR	B	91	41.563	8.271	93.226	1.00	29.27
ATOM	3750	O	TYR	B	91	42.109	8.874	92.308	1.00	25.22
ATOM	3751	N	GLU	B	92	41.568	6.948	93.318	1.00	28.32
ATOM	3752	CA	GLU	B	92	42.286	6.124	92.350	1.00	27.06
ATOM	3753	CB	GLU	B	92	42.474	4.726	92.924	1.00	23.35
ATOM	3754	CG	GLU	B	92	43.502	3.884	92.221	1.00	29.80
ATOM	3755	CD	GLU	B	92	43.585	2.500	92.826	1.00	35.34
ATOM	3756	OE1	GLU	B	92	42.742	1.645	92.477	1.00	32.15
ATOM	3757	OE2	GLU	B	92	44.475	2.278	93.678	1.00	31.61
ATOM	3758	C	GLU	B	92	41.594	6.024	90.997	1.00	23.42
ATOM	3759	O	GLU	B	92	42.204	6.260	89.962	1.00	20.47
ATOM	3760	N	ASN	B	93	40.314	5.677	91.017	1.00	18.85
ATOM	3761	CA	ASN	B	93	39.534	5.509	89.795	1.00	21.96
ATOM	3762	CB	ASN	B	93	39.165	4.033	89.664	1.00	23.90
ATOM	3763	CG	ASN	B	93	40.351	3.120	89.943	1.00	24.78
ATOM	3764	OD1	ASN	B	93	41.362	3.160	89.239	1.00	22.35
ATOM	3765	ND2	ASN	B	93	40.240	2.311	90.987	1.00	13.35
ATOM	3766	C	ASN	B	93	38.285	6.362	89.944	1.00	25.16
ATOM	3767	O	ASN	B	93	37.183	5.843	90.121	1.00	20.91
ATOM	3768	N	PRO	B	94	38.449	7.693	89.887	1.00	26.37
ATOM	3769	CD	PRO	B	94	39.738	8.389	89.716	1.00	19.35
ATOM	3770	CA	PRO	B	94	37.373	8.676	90.024	1.00	24.59
ATOM	3771	CB	PRO	B	94	38.147	9.972	90.200	1.00	25.95
ATOM	3772	CG	PRO	B	94	39.297	9.740	89.223	1.00	22.60
ATOM	3773	C	PRO	B	94	36.384	8.777	88.873	1.00	28.74
ATOM	3774	O	PRO	B	94	36.562	8.176	87.808	1.00	25.77
ATOM	3775	N	VAL	B	95	35.332	9.553	89.112	1.00	27.14
ATOM	3776	CA	VAL	B	95	34.317	9.812	88.103	1.00	25.94
ATOM	3777	CB	VAL	B	95	33.035	10.393	88.742	1.00	23.75
ATOM	3778	CG1	VAL	B	95	32.067	10.855	87.662	1.00	26.34
ATOM	3779	CG2	VAL	B	95	32.378	9.346	89.622	1.00	27.59
ATOM	3780	C	VAL	B	95	34.912	10.861	87.175	1.00	25.69
ATOM	3781	O	VAL	B	95	35.564	11.793	87.641	1.00	25.25
ATOM	3782	N	SER	B	96	34.708	10.699	85.871	1.00	28.02
ATOM	3783	CA	SER	B	96	35.199	11.647	84.868	1.00	24.82
ATOM	3784	CB	SER	B	96	36.729	11.705	84.850	1.00	25.90
ATOM	3785	OG	SER	B	96	37.274	10.548	84.229	1.00	23.99

174/263

Figure 18-58

ATOM	3786	C	SER	B	96	34.726	11.127	83.519	1.00	26.22
ATOM	3787	O	SER	B	96	33.943	10.174	83.462	1.00	23.57
ATOM	3788	N	TYR	B	97	35.195	11.744	82.438	1.00	22.83
ATOM	3789	CA	TYR	B	97	34.818	11.279	81.110	1.00	28.59
ATOM	3790	CB	TYR	B	97	34.536	12.452	80.165	1.00	31.45
ATOM	3791	CG	TYR	B	97	33.279	13.203	80.548	1.00	35.09
ATOM	3792	CD1	TYR	B	97	33.316	14.239	81.480	1.00	32.87
ATOM	3793	CE1	TYR	B	97	32.148	14.863	81.911	1.00	37.73
ATOM	3794	CD2	TYR	B	97	32.036	12.812	80.049	1.00	34.85
ATOM	3795	CE2	TYR	B	97	30.858	13.430	80.475	1.00	38.61
ATOM	3796	CZ	TYR	B	97	30.924	14.453	81.408	1.00	39.45
ATOM	3797	OH	TYR	B	97	29.768	15.047	81.852	1.00	35.36
ATOM	3798	C	TYR	B	97	35.883	10.354	80.534	1.00	28.93
ATOM	3799	O	TYR	B	97	35.859	9.992	79.358	1.00	28.26
ATOM	3800	N	ALA	B	98	36.822	9.968	81.385	1.00	29.09
ATOM	3801	CA	ALA	B	98	37.866	9.044	80.980	1.00	26.88
ATOM	3802	CB	ALA	B	98	39.167	9.369	81.692	1.00	27.99
ATOM	3803	C	ALA	B	98	37.395	7.657	81.382	1.00	22.53
ATOM	3804	O	ALA	B	98	37.721	6.675	80.722	1.00	21.98
ATOM	3805	N	MET	B	99	36.603	7.595	82.453	1.00	23.51
ATOM	3806	CA	MET	B	99	36.106	6.326	82.986	1.00	26.36
ATOM	3807	CB	MET	B	99	35.179	6.568	84.185	1.00	24.05
ATOM	3808	CG	MET	B	99	33.822	7.188	83.875	1.00	28.37
ATOM	3809	SD	MET	B	99	32.966	7.704	85.406	1.00	27.91
ATOM	3810	CE	MET	B	99	33.106	6.227	86.409	1.00	22.12
ATOM	3811	C	MET	B	99	35.430	5.435	81.953	1.00	25.76
ATOM	3812	O	MET	B	99	35.544	4.212	82.031	1.00	26.11
ATOM	3813	N	PHE	B	100	34.724	6.027	80.992	1.00	22.17
ATOM	3814	CA	PHE	B	100	34.107	5.222	79.940	1.00	22.35
ATOM	3815	CB	PHE	B	100	32.582	5.133	80.088	1.00	22.01
ATOM	3816	CG	PHE	B	100	31.947	4.254	79.038	1.00	24.22
ATOM	3817	CD1	PHE	B	100	32.143	2.872	79.061	1.00	26.61
ATOM	3818	CD2	PHE	B	100	31.280	4.813	77.953	1.00	21.22
ATOM	3819	CE1	PHE	B	100	31.691	2.059	78.012	1.00	26.91
ATOM	3820	CE2	PHE	B	100	30.825	4.010	76.894	1.00	24.80
ATOM	3821	CZ	PHE	B	100	31.033	2.632	76.924	1.00	24.85
ATOM	3822	C	PHE	B	100	34.425	5.695	78.514	1.00	24.86
ATOM	3823	O	PHE	B	100	34.922	4.920	77.694	1.00	21.40
ATOM	3824	N	THR	B	101	34.131	6.957	78.204	1.00	24.24
ATOM	3825	CA	THR	B	101	34.390	7.469	76.854	1.00	24.54
ATOM	3826	CB	THR	B	101	33.914	8.926	76.708	1.00	24.46
ATOM	3827	OG1	THR	B	101	32.504	8.985	76.953	1.00	27.64
ATOM	3828	CG2	THR	B	101	34.191	9.445	75.297	1.00	22.19
ATOM	3829	C	THR	B	101	35.872	7.387	76.483	1.00	25.26
ATOM	3830	O	THR	B	101	36.231	6.856	75.430	1.00	25.47
ATOM	3831	N	GLY	B	102	36.725	7.916	77.350	1.00	23.74
ATOM	3832	CA	GLY	B	102	38.153	7.867	77.096	1.00	24.53
ATOM	3833	C	GLY	B	102	38.657	6.434	77.046	1.00	24.06
ATOM	3834	O	GLY	B	102	39.346	6.045	76.100	1.00	22.53
ATOM	3835	N	SER	B	103	38.316	5.651	78.067	1.00	22.02
ATOM	3836	CA	SER	B	103	38.730	4.253	78.146	1.00	20.45
ATOM	3837	CB	SER	B	103	38.193	3.613	79.427	1.00	25.21
ATOM	3838	OG	SER	B	103	38.820	4.166	80.567	1.00	26.48
ATOM	3839	C	SER	B	103	38.268	3.446	76.938	1.00	20.53
ATOM	3840	O	SER	B	103	39.034	2.669	76.372	1.00	16.82
ATOM	3841	N	SER	B	104	37.014	3.642	76.542	1.00	17.11
ATOM	3842	CA	SER	B	104	36.462	2.937	75.395	1.00	23.32
ATOM	3843	CB	SER	B	104	34.980	3.289	75.228	1.00	22.93
ATOM	3844	OG	SER	B	104	34.424	2.557	74.161	1.00	24.75
ATOM	3845	C	SER	B	104	37.221	3.288	74.116	1.00	21.97
ATOM	3846	O	SER	B	104	37.451	2.434	73.256	1.00	22.83
ATOM	3847	N	LEU	B	105	37.619	4.549	73.997	1.00	23.00
ATOM	3848	CA	LEU	B	105	38.354	5.007	72.825	1.00	25.12
ATOM	3849	CB	LEU	B	105	38.443	6.536	72.859	1.00	29.25
ATOM	3850	CG	LEU	B	105	38.702	7.289	71.553	1.00	34.27
ATOM	3851	CD1	LEU	B	105	37.662	6.888	70.512	1.00	31.51

175/263

Figure 18-59

ATOM	3852	CD2	LEU B 105	38.629	8.802	71.819	1.00	34.30
ATOM	3853	C	LEU B 105	39.755	4.374	72.813	1.00	27.39
ATOM	3854	O	LEU B 105	40.262	3.955	71.765	1.00	20.15
ATOM	3855	N	ALA B 106	40.371	4.293	73.988	1.00	23.62
ATOM	3856	CA	ALA B 106	41.704	3.692	74.115	1.00	22.73
ATOM	3857	CB	ALA B 106	42.263	3.939	75.529	1.00	17.46
ATOM	3858	C	ALA B 106	41.639	2.189	73.846	1.00	22.77
ATOM	3859	O	ALA B 106	42.583	1.597	73.316	1.00	24.98
ATOM	3860	N	THR B 107	40.523	1.567	74.224	1.00	23.54
ATOM	3861	CA	THR B 107	40.355	0.132	74.033	1.00	19.76
ATOM	3862	CB	THR B 107	39.236	-0.410	74.947	1.00	22.85
ATOM	3863	OG1	THR B 107	39.572	-0.128	76.306	1.00	16.29
ATOM	3864	CG2	THR B 107	39.085	-1.917	74.787	1.00	17.21
ATOM	3865	C	THR B 107	40.036	-0.169	72.571	1.00	23.47
ATOM	3866	O	THR B 107	40.540	-1.138	72.001	1.00	19.25
ATOM	3867	N	GLY B 108	39.191	0.656	71.959	1.00	24.87
ATOM	3868	CA	GLY B 108	38.879	0.434	70.560	1.00	21.32
ATOM	3869	C	GLY B 108	40.161	0.594	69.757	1.00	22.01
ATOM	3870	O	GLY B 108	40.388	-0.099	68.761	1.00	20.46
ATOM	3871	N	SER B 109	41.018	1.508	70.197	1.00	19.89
ATOM	3872	CA	SER B 109	42.274	1.749	69.499	1.00	19.37
ATOM	3873	CB	SER B 109	42.993	2.956	70.107	1.00	18.28
ATOM	3874	OG	SER B 109	42.250	4.145	69.882	1.00	21.29
ATOM	3875	C	SER B 109	43.168	0.513	69.542	1.00	20.70
ATOM	3876	O	SER B 109	43.940	0.261	68.617	1.00	20.69
ATOM	3877	N	THR B 110	43.065	-0.259	70.616	1.00	20.54
ATOM	3878	CA	THR B 110	43.858	-1.475	70.729	1.00	19.98
ATOM	3879	CB	THR B 110	43.826	-2.043	72.158	1.00	20.63
ATOM	3880	OG1	THR B 110	44.632	-1.215	73.007	1.00	20.72
ATOM	3881	CG2	THR B 110	44.371	-3.470	72.188	1.00	20.05
ATOM	3882	C	THR B 110	43.333	-2.507	69.738	1.00	21.61
ATOM	3883	O	THR B 110	44.115	-3.239	69.127	1.00	18.11
ATOM	3884	N	VAL B 111	42.012	-2.557	69.567	1.00	18.29
ATOM	3885	CA	VAL B 111	41.432	-3.486	68.608	1.00	20.36
ATOM	3886	CB	VAL B 111	39.886	-3.494	68.677	1.00	23.94
ATOM	3887	CG1	VAL B 111	39.324	-4.442	67.619	1.00	24.37
ATOM	3888	CG2	VAL B 111	39.426	-3.937	70.063	1.00	21.60
ATOM	3889	C	VAL B 111	41.872	-3.080	67.197	1.00	20.35
ATOM	3890	O	VAL B 111	42.146	-3.936	66.362	1.00	23.29
ATOM	3891	N	GLN B 112	41.953	-1.775	66.937	1.00	22.07
ATOM	3892	CA	GLN B 112	42.367	-1.290	65.617	1.00	22.34
ATOM	3893	CB	GLN B 112	42.199	0.230	65.513	1.00	24.54
ATOM	3894	CG	GLN B 112	40.810	0.729	65.843	1.00	20.63
ATOM	3895	CD	GLN B 112	40.700	2.236	65.742	1.00	21.19
ATOM	3896	OE1	GLN B 112	40.664	2.794	64.645	1.00	26.73
ATOM	3897	NE2	GLN B 112	40.667	2.905	66.886	1.00	18.73
ATOM	3898	C	GLN B 112	43.826	-1.635	65.363	1.00	23.11
ATOM	3899	O	GLN B 112	44.195	-2.020	64.257	1.00	15.79
ATOM	3900	N	ALA B 113	44.660	-1.476	66.389	1.00	20.60
ATOM	3901	CA	ALA B 113	46.070	-1.790	66.249	1.00	18.02
ATOM	3902	CB	ALA B 113	46.794	-1.536	67.548	1.00	20.84
ATOM	3903	C	ALA B 113	46.170	-3.262	65.863	1.00	23.78
ATOM	3904	O	ALA B 113	46.982	-3.642	65.023	1.00	19.53
ATOM	3905	N	ILE B 114	45.331	-4.091	66.477	1.00	21.45
ATOM	3906	CA	ILE B 114	45.344	-5.511	66.168	1.00	24.26
ATOM	3907	CB	ILE B 114	44.507	-6.306	67.191	1.00	20.72
ATOM	3908	CG2	ILE B 114	44.476	-7.779	66.800	1.00	21.92
ATOM	3909	CG1	ILE B 114	45.116	-6.144	68.593	1.00	24.32
ATOM	3910	CD1	ILE B 114	44.364	-6.872	69.694	1.00	19.01
ATOM	3911	C	ILE B 114	44.808	-5.765	64.753	1.00	26.75
ATOM	3912	O	ILE B 114	45.305	-6.640	64.032	1.00	20.18
ATOM	3913	N	GLU B 115	43.792	-5.009	64.347	1.00	24.69
ATOM	3914	CA	GLU B 115	43.243	-5.198	63.005	1.00	29.26
ATOM	3915	CB	GLU B 115	42.043	-4.278	62.770	1.00	29.07
ATOM	3916	CG	GLU B 115	40.940	-4.421	63.800	1.00	32.31
ATOM	3917	CD	GLU B 115	39.757	-3.519	63.516	1.00	38.14

Figure 18-60

ATOM	3918	OE1	GLU	B	115	39.980	-2.374	63.072	1.00	40.63
ATOM	3919	OE2	GLU	B	115	38.607	-3.940	63.758	1.00	39.86
ATOM	3920	C	GLU	B	115	44.334	-4.906	61.974	1.00	31.52
ATOM	3921	O	GLU	B	115	44.444	-5.603	60.964	1.00	26.43
ATOM	3922	N	GLU	B	116	45.141	-3.879	62.234	1.00	26.04
ATOM	3923	CA	GLU	B	116	46.226	-3.522	61.324	1.00	26.21
ATOM	3924	CB	GLU	B	116	46.909	-2.227	61.775	1.00	23.21
ATOM	3925	CG	GLU	B	116	46.055	-0.983	61.601	1.00	23.82
ATOM	3926	CD	GLU	B	116	45.576	-0.817	60.163	1.00	31.43
ATOM	3927	OE1	GLU	B	116	46.425	-0.734	59.253	1.00	26.45
ATOM	3928	OE2	GLU	B	116	44.349	-0.771	59.945	1.00	24.59
ATOM	3929	C	GLU	B	116	47.256	-4.644	61.243	1.00	28.60
ATOM	3930	O	GLU	B	116	47.857	-4.884	60.189	1.00	25.01
ATOM	3931	N	PHE	B	117	47.470	-5.324	62.363	1.00	26.22
ATOM	3932	CA	PHE	B	117	48.421	-6.425	62.400	1.00	28.05
ATOM	3933	CB	PHE	B	117	48.516	-7.007	63.805	1.00	32.15
ATOM	3934	CG	PHE	B	117	49.278	-8.299	63.869	1.00	33.88
ATOM	3935	CD1	PHE	B	117	50.656	-8.321	63.713	1.00	33.52
ATOM	3936	CD2	PHE	B	117	48.604	-9.502	64.054	1.00	32.83
ATOM	3937	CE1	PHE	B	117	51.356	-9.521	63.740	1.00	31.67
ATOM	3938	CE2	PHE	B	117	49.294	-10.710	64.082	1.00	35.69
ATOM	3939	CZ	PHE	B	117	50.674	-10.717	63.926	1.00	36.72
ATOM	3940	C	PHE	B	117	47.929	-7.508	61.456	1.00	26.43
ATOM	3941	O	PHE	B	117	48.689	-8.061	60.669	1.00	27.61
ATOM	3942	N	LEU	B	118	46.642	-7.809	61.551	1.00	23.59
ATOM	3943	CA	LEU	B	118	46.048	-8.820	60.705	1.00	29.15
ATOM	3944	CB	LEU	B	118	44.585	-9.039	61.099	1.00	28.78
ATOM	3945	CG	LEU	B	118	44.375	-9.478	62.557	1.00	35.24
ATOM	3946	CD1	LEU	B	118	42.898	-9.763	62.788	1.00	31.92
ATOM	3947	CD2	LEU	B	118	45.205	-10.723	62.856	1.00	33.40
ATOM	3948	C	LEU	B	118	46.153	-8.422	59.236	1.00	30.15
ATOM	3949	O	LEU	B	118	46.350	-9.276	58.379	1.00	27.04
ATOM	3950	N	LYS	B	119	46.035	-7.128	58.947	1.00	27.96
ATOM	3951	CA	LYS	B	119	46.127	-6.663	57.569	1.00	26.69
ATOM	3952	CB	LYS	B	119	45.470	-5.291	57.412	1.00	23.94
ATOM	3953	CG	LYS	B	119	43.998	-5.260	57.795	1.00	24.41
ATOM	3954	CD	LYS	B	119	43.327	-3.970	57.350	1.00	27.53
ATOM	3955	CE	LYS	B	119	44.024	-2.739	57.886	1.00	33.13
ATOM	3956	NZ	LYS	B	119	43.371	-1.479	57.428	1.00	27.75
ATOM	3957	C	LYS	B	119	47.577	-6.598	57.101	1.00	29.12
ATOM	3958	O	LYS	B	119	47.864	-6.160	55.984	1.00	35.25
ATOM	3959	N	GLY	B	120	48.493	-7.034	57.958	1.00	30.25
ATOM	3960	CA	GLY	B	120	49.896	-7.037	57.585	1.00	28.38
ATOM	3961	C	GLY	B	120	50.642	-5.751	57.861	1.00	27.91
ATOM	3962	O	GLY	B	120	51.775	-5.582	57.403	1.00	22.25
ATOM	3963	N	ASN	B	121	50.024	-4.836	58.600	1.00	25.42
ATOM	3964	CA	ASN	B	121	50.695	-3.587	58.919	1.00	29.49
ATOM	3965	CB	ASN	B	121	49.758	-2.389	58.727	1.00	30.07
ATOM	3966	CG	ASN	B	121	49.201	-2.307	57.325	1.00	32.25
ATOM	3967	OD1	ASN	B	121	49.924	-2.491	56.350	1.00	35.44
ATOM	3968	ND2	ASN	B	121	47.917	-2.006	57.217	1.00	32.26
ATOM	3969	C	ASN	B	121	51.172	-3.637	60.361	1.00	30.92
ATOM	3970	O	ASN	B	121	50.971	-4.631	61.059	1.00	27.08
ATOM	3971	N	VAL	B	122	51.810	-2.560	60.796	1.00	28.46
ATOM	3972	CA	VAL	B	122	52.309	-2.457	62.155	1.00	29.48
ATOM	3973	CB	VAL	B	122	53.840	-2.352	62.177	1.00	33.40
ATOM	3974	CG1	VAL	B	122	54.334	-2.294	63.611	1.00	32.22
ATOM	3975	CG2	VAL	B	122	54.446	-3.544	61.458	1.00	33.57
ATOM	3976	C	VAL	B	122	51.713	-1.196	62.748	1.00	29.04
ATOM	3977	O	VAL	B	122	51.800	-0.118	62.153	1.00	27.47
ATOM	3978	N	ALA	B	123	51.100	-1.326	63.918	1.00	26.71
ATOM	3979	CA	ALA	B	123	50.477	-0.177	64.559	1.00	25.62
ATOM	3980	CB	ALA	B	123	48.963	-0.281	64.447	1.00	21.65
ATOM	3981	C	ALA	B	123	50.872	-0.005	66.017	1.00	28.62
ATOM	3982	O	ALA	B	123	51.227	-0.965	66.712	1.00	26.96
ATOM	3983	N	PHE	B	124	50.805	1.239	66.472	1.00	22.85

Figure 18-61

ATOM	3984	CA	PHE	B	124	51.122	1.577	67.847	1.00	17.31
ATOM	3985	CB	PHE	B	124	52.419	2.404	67.876	1.00	16.88
ATOM	3986	CG	PHE	B	124	52.762	3.000	69.225	1.00	18.52
ATOM	3987	CD1	PHE	B	124	52.533	2.304	70.403	1.00	17.52
ATOM	3988	CD2	PHE	B	124	53.382	4.245	69.297	1.00	17.88
ATOM	3989	CE1	PHE	B	124	52.914	2.837	71.638	1.00	25.77
ATOM	3990	CE2	PHE	B	124	53.769	4.790	70.517	1.00	21.97
ATOM	3991	CZ	PHE	B	124	53.535	4.084	71.698	1.00	20.16
ATOM	3992	C	PHE	B	124	49.937	2.348	68.421	1.00	18.77
ATOM	3993	O	PHE	B	124	49.462	3.311	67.820	1.00	16.62
ATOM	3994	N	ASN	B	125	49.418	1.868	69.546	1.00	16.69
ATOM	3995	CA	ASN	B	125	48.320	2.528	70.238	1.00	16.22
ATOM	3996	CB	ASN	B	125	47.129	1.603	70.435	1.00	12.71
ATOM	3997	CG	ASN	B	125	46.095	2.209	71.346	1.00	19.79
ATOM	3998	OD1	ASN	B	125	45.930	3.430	71.372	1.00	20.83
ATOM	3999	ND2	ASN	B	125	45.376	1.371	72.087	1.00	12.31
ATOM	4000	C	ASN	B	125	48.790	3.004	71.600	1.00	19.19
ATOM	4001	O	ASN	B	125	48.687	2.280	72.585	1.00	20.99
ATOM	4002	N	PRO	B	126	49.335	4.226	71.668	1.00	19.02
ATOM	4003	CD	PRO	B	126	49.595	5.156	70.555	1.00	21.39
ATOM	4004	CA	PRO	B	126	49.833	4.805	72.917	1.00	21.60
ATOM	4005	CB	PRO	B	126	50.398	6.161	72.459	1.00	21.07
ATOM	4006	CG	PRO	B	126	49.530	6.487	71.269	1.00	17.70
ATOM	4007	C	PRO	B	126	48.808	4.942	74.034	1.00	20.69
ATOM	4008	O	PRO	B	126	49.178	5.053	75.198	1.00	19.79
ATOM	4009	N	ALA	B	127	47.525	4.937	73.689	1.00	16.67
ATOM	4010	CA	ALA	B	127	46.476	5.065	74.698	1.00	20.44
ATOM	4011	CB	ALA	B	127	45.198	5.609	74.066	1.00	19.56
ATOM	4012	C	ALA	B	127	46.169	3.747	75.401	1.00	20.80
ATOM	4013	O	ALA	B	127	45.555	3.742	76.472	1.00	19.47
ATOM	4014	N	GLY	B	128	46.587	2.634	74.800	1.00	20.52
ATOM	4015	CA	GLY	B	128	46.325	1.333	75.399	1.00	19.43
ATOM	4016	C	GLY	B	128	47.327	0.910	76.463	1.00	20.56
ATOM	4017	O	GLY	B	128	48.182	1.697	76.869	1.00	18.37
ATOM	4018	N	GLY	B	129	47.215	-0.333	76.929	1.00	19.68
ATOM	4019	CA	GLY	B	129	48.136	-0.820	77.943	1.00	19.93
ATOM	4020	C	GLY	B	129	47.620	-0.619	79.358	1.00	25.25
ATOM	4021	O	GLY	B	129	48.383	-0.686	80.329	1.00	18.98
ATOM	4022	N	MET	B	130	46.317	-0.374	79.474	1.00	16.04
ATOM	4023	CA	MET	B	130	45.677	-0.161	80.768	1.00	19.26
ATOM	4024	CB	MET	B	130	44.301	0.451	80.519	1.00	17.94
ATOM	4025	CG	MET	B	130	44.413	1.728	79.653	1.00	22.95
ATOM	4026	SD	MET	B	130	42.873	2.615	79.307	1.00	31.83
ATOM	4027	CE	MET	B	130	41.957	1.358	78.382	1.00	20.22
ATOM	4028	C	MET	B	130	45.598	-1.548	81.421	1.00	22.63
ATOM	4029	O	MET	B	130	44.546	-2.173	81.486	1.00	16.24
ATOM	4030	N	HIS	B	131	46.737	-1.999	81.932	1.00	18.42
ATOM	4031	CA	HIS	B	131	46.853	-3.343	82.472	1.00	17.07
ATOM	4032	CB	HIS	B	131	48.323	-3.804	82.341	1.00	17.61
ATOM	4033	CG	HIS	B	131	49.316	-2.979	83.106	1.00	14.01
ATOM	4034	CD2	HIS	B	131	49.138	-1.904	83.915	1.00	13.47
ATOM	4035	ND1	HIS	B	131	50.680	-3.190	83.051	1.00	18.00
ATOM	4036	CE1	HIS	B	131	51.297	-2.281	83.789	1.00	15.27
ATOM	4037	NE2	HIS	B	131	50.384	-1.489	84.324	1.00	17.21
ATOM	4038	C	HIS	B	131	46.329	-3.724	83.852	1.00	16.41
ATOM	4039	O	HIS	B	131	46.452	-4.883	84.236	1.00	19.37
ATOM	4040	N	HIS	B	132	45.721	-2.794	84.586	1.00	18.64
ATOM	4041	CA	HIS	B	132	45.241	-3.112	85.936	1.00	20.87
ATOM	4042	CB	HIS	B	132	45.513	-1.935	86.885	1.00	18.85
ATOM	4043	CG	HIS	B	132	46.966	-1.686	87.152	1.00	20.00
ATOM	4044	CD2	HIS	B	132	47.715	-0.563	87.030	1.00	15.74
ATOM	4045	ND1	HIS	B	132	47.810	-2.655	87.659	1.00	14.72
ATOM	4046	CE1	HIS	B	132	49.014	-2.139	87.837	1.00	14.64
ATOM	4047	NE2	HIS	B	132	48.984	-0.872	87.462	1.00	14.88
ATOM	4048	C	HIS	B	132	43.778	-3.547	86.136	1.00	22.83
ATOM	4049	O	HIS	B	132	43.478	-4.298	87.076	1.00	17.84

ATOM	4050	N	ALA	B	133	42.878	-3.088	85.271	1.00	16.54
ATOM	4051	CA	ALA	B	133	41.457	-3.396	85.424	1.00	19.13
ATOM	4052	CB	ALA	B	133	40.654	-2.704	84.328	1.00	23.56
ATOM	4053	C	ALA	B	133	41.127	-4.883	85.439	1.00	23.12
ATOM	4054	O	ALA	B	133	41.718	-5.677	84.696	1.00	18.03
ATOM	4055	N	PHE	B	134	40.181	-5.257	86.294	1.00	19.69
ATOM	4056	CA	PHE	B	134	39.762	-6.649	86.365	1.00	19.35
ATOM	4057	CB	PHE	B	134	39.583	-7.122	87.818	1.00	21.26
ATOM	4058	CG	PHE	B	134	40.837	-7.053	88.646	1.00	23.41
ATOM	4059	CD1	PHE	B	134	41.041	-6.009	89.544	1.00	24.25
ATOM	4060	CD2	PHE	B	134	41.820	-8.027	88.522	1.00	22.80
ATOM	4061	CE1	PHE	B	134	42.207	-5.935	90.311	1.00	23.36
ATOM	4062	CE2	PHE	B	134	42.997	-7.964	89.283	1.00	27.74
ATOM	4063	CZ	PHE	B	134	43.190	-6.917	90.178	1.00	24.05
ATOM	4064	C	PHE	B	134	38.444	-6.816	85.621	1.00	18.60
ATOM	4065	O	PHE	B	134	37.815	-5.849	85.196	1.00	13.82
ATOM	4066	N	LYS	B	135	38.050	-8.064	85.454	1.00	19.78
ATOM	4067	CA	LYS	B	135	36.813	-8.421	84.782	1.00	28.09
ATOM	4068	CB	LYS	B	135	36.501	-9.879	85.125	1.00	34.06
ATOM	4069	CG	LYS	B	135	35.077	-10.310	84.953	1.00	42.76
ATOM	4070	CD	LYS	B	135	34.927	-11.745	85.437	1.00	48.44
ATOM	4071	CE	LYS	B	135	33.462	-12.152	85.531	1.00	55.66
ATOM	4072	NZ	LYS	B	135	32.727	-11.332	86.544	1.00	51.65
ATOM	4073	C	LYS	B	135	35.639	-7.512	85.172	1.00	28.27
ATOM	4074	O	LYS	B	135	34.927	-6.999	84.309	1.00	24.86
ATOM	4075	N	SER	B	136	35.450	-7.292	86.470	1.00	29.89
ATOM	4076	CA	SER	B	136	34.331	-6.477	86.933	1.00	30.86
ATOM	4077	CB	SER	B	136	33.282	-7.388	87.582	1.00	31.57
ATOM	4078	OG	SER	B	136	32.916	-8.434	86.698	1.00	45.10
ATOM	4079	C	SER	B	136	34.705	-5.380	87.923	1.00	31.50
ATOM	4080	O	SER	B	136	33.887	-4.997	88.765	1.00	24.54
ATOM	4081	N	ARG	B	137	35.920	-4.854	87.835	1.00	22.63
ATOM	4082	CA	ARG	B	137	36.291	-3.826	88.794	1.00	25.51
ATOM	4083	CB	ARG	B	137	36.629	-4.486	90.136	1.00	29.62
ATOM	4084	CG	ARG	B	137	36.391	-3.578	91.318	1.00	36.21
ATOM	4085	CD	ARG	B	137	36.874	-4.160	92.631	1.00	40.79
ATOM	4086	NE	ARG	B	137	36.365	-3.357	93.744	1.00	45.95
ATOM	4087	CZ	ARG	B	137	36.863	-3.369	94.973	1.00	41.97
ATOM	4088	NH1	ARG	B	137	37.897	-4.144	95.263	1.00	43.42
ATOM	4089	NH2	ARG	B	137	36.322	-2.604	95.913	1.00	46.65
ATOM	4090	C	ARG	B	137	37.461	-2.956	88.339	1.00	24.73
ATOM	4091	O	ARG	B	137	38.420	-3.441	87.734	1.00	19.32
ATOM	4092	N	ALA	B	138	37.372	-1.663	88.631	1.00	16.77
ATOM	4093	CA	ALA	B	138	38.428	-0.733	88.270	1.00	18.50
ATOM	4094	CB	ALA	B	138	37.939	0.694	88.401	1.00	17.24
ATOM	4095	C	ALA	B	138	39.597	-0.964	89.216	1.00	22.62
ATOM	4096	O	ALA	B	138	39.411	-1.419	90.346	1.00	18.98
ATOM	4097	N	ASN	B	139	40.301	-0.641	88.759	1.00	20.82
ATOM	4098	CA	ASN	B	139	41.989	-0.828	89.585	1.00	25.17
ATOM	4099	CB	ASN	B	139	42.311	-2.329	89.689	1.00	20.59
ATOM	4100	CG	ASN	B	139	43.556	-2.608	90.511	1.00	27.70
ATOM	4101	OD1	ASN	B	139	43.726	-2.057	91.592	1.00	22.43
ATOM	4102	ND2	ASN	B	139	44.420	-3.487	90.010	1.00	24.43
ATOM	4103	C	ASN	B	139	43.176	-0.062	89.020	1.00	22.37
ATOM	4104	O	ASN	B	139	43.338	0.038	87.799	1.00	17.50
ATOM	4105	N	GLY	B	140	43.984	0.496	89.920	1.00	21.67
ATOM	4106	CA	GLY	B	140	45.166	1.249	89.524	1.00	23.06
ATOM	4107	C	GLY	B	140	45.005	2.268	88.402	1.00	26.29
ATOM	4108	O	GLY	B	140	45.827	2.301	87.479	1.00	22.47
ATOM	4109	N	PHE	B	141	43.958	3.093	88.473	1.00	22.33
ATOM	4110	CA	PHE	B	141	43.694	4.126	87.461	1.00	19.01
ATOM	4111	CB	PHE	B	141	44.996	4.806	86.997	1.00	22.90
ATOM	4112	CG	PHE	B	141	45.810	5.433	88.097	1.00	23.17
ATOM	4113	CD1	PHE	B	141	47.114	5.851	87.842	1.00	22.17
ATOM	4114	CD2	PHE	B	141	45.281	5.635	89.366	1.00	23.40
ATOM	4115	CE1	PHE	B	141	47.876	6.462	88.833	1.00	24.02

ATOM	4116	CE2	PHE	B	141	46.033	6.244	90.361	1.00	23.03
ATOM	4117	CZ	PHE	B	141	47.335	6.658	90.092	1.00	25.15
ATOM	4118	C	PHE	B	141	43.029	3.538	86.214	1.00	23.69
ATOM	4119	O	PHE	B	141	42.596	4.283	85.335	1.00	18.88
ATOM	4120	N	CYS	B	142	42.962	2.211	86.122	1.00	15.03
ATOM	4121	CA	CYS	B	142	42.380	1.578	84.938	1.00	19.55
ATOM	4122	CB	CYS	B	142	43.193	0.336	84.552	1.00	20.38
ATOM	4123	SG	CYS	B	142	44.933	0.662	84.190	1.00	37.40
ATOM	4124	C	CYS	B	142	40.923	1.171	85.098	1.00	22.77
ATOM	4125	O	CYS	B	142	40.561	0.514	86.082	1.00	23.04
ATOM	4126	N	TYR	B	143	40.094	1.557	84.130	1.00	15.24
ATOM	4127	CA	TYR	B	143	38.675	1.194	84.155	1.00	21.97
ATOM	4128	CB	TYR	B	143	37.795	2.372	83.723	1.00	18.06
ATOM	4129	CG	TYR	B	143	38.016	3.622	84.535	1.00	24.34
ATOM	4130	CD1	TYR	B	143	39.038	4.516	84.214	1.00	23.20
ATOM	4131	CE1	TYR	B	143	39.265	5.658	84.991	1.00	27.42
ATOM	4132	CD2	TYR	B	143	37.226	3.892	85.652	1.00	19.15
ATOM	4133	CE2	TYR	B	143	37.441	5.023	86.432	1.00	21.92
ATOM	4134	CZ	TYR	B	143	38.458	5.900	86.099	1.00	23.94
ATOM	4135	OH	TYR	B	143	38.655	7.015	86.877	1.00	22.37
ATOM	4136	C	TYR	B	143	38.431	0.008	83.218	1.00	19.91
ATOM	4137	O	TYR	B	143	37.665	-0.902	83.535	1.00	22.50
ATOM	4138	N	ILE	B	144	39.083	0.026	82.061	1.00	19.20
ATOM	4139	CA	ILE	B	144	38.938	-1.055	81.082	1.00	19.68
ATOM	4140	CB	ILE	B	144	38.282	-0.528	79.787	1.00	20.26
ATOM	4141	CG2	ILE	B	144	38.151	-1.649	78.760	1.00	15.37
ATOM	4142	CG1	ILE	B	144	36.901	0.053	80.113	1.00	20.93
ATOM	4143	CD1	ILE	B	144	36.198	0.697	78.917	1.00	23.75
ATOM	4144	C	ILE	B	144	40.320	-1.627	80.774	1.00	22.78
ATOM	4145	O	ILE	B	144	41.281	-0.873	80.600	1.00	22.01
ATOM	4146	N	ASN	B	145	40.422	-2.956	80.723	1.00	23.18
ATOM	4147	CA	ASN	B	145	41.698	-3.623	80.451	1.00	20.63
ATOM	4148	CB	ASN	B	145	41.778	-4.935	81.243	1.00	17.81
ATOM	4149	CG	ASN	B	145	43.188	-5.531	81.268	1.00	25.17
ATOM	4150	OD1	ASN	B	145	43.804	-5.742	80.227	1.00	23.63
ATOM	4151	ND2	ASN	B	145	43.693	-5.819	82.472	1.00	22.69
ATOM	4152	C	ASN	B	145	41.780	-3.918	78.955	1.00	21.18
ATOM	4153	O	ASN	B	145	41.389	-5.002	78.508	1.00	17.80
ATOM	4154	N	ASN	B	146	42.293	-2.968	78.177	1.00	15.23
ATOM	4155	CA	ASN	B	146	42.367	-3.175	76.733	1.00	19.71
ATOM	4156	CB	ASN	B	146	42.773	-1.880	76.015	1.00	17.65
ATOM	4157	CG	ASN	B	146	44.196	-1.458	76.306	1.00	19.86
ATOM	4158	OD1	ASN	B	146	45.109	-1.735	75.532	1.00	20.27
ATOM	4159	ND2	ASN	B	146	44.395	-0.798	77.435	1.00	11.85
ATOM	4160	C	ASN	B	146	43.277	-4.342	76.331	1.00	19.07
ATOM	4161	O	ASN	B	146	43.030	-4.996	75.328	1.00	18.61
ATOM	4162	N	PRO	B	147	44.358	-4.598	77.082	1.00	17.78
ATOM	4163	CD	PRO	B	147	44.953	-3.919	78.240	1.00	18.13
ATOM	4164	CA	PRO	B	147	45.197	-5.735	76.678	1.00	19.98
ATOM	4165	CB	PRO	B	147	46.338	-5.694	77.698	1.00	24.29
ATOM	4166	CG	PRO	B	147	46.425	-4.201	78.020	1.00	26.27
ATOM	4167	C	PRO	B	147	44.377	-7.041	76.757	1.00	20.91
ATOM	4168	O	PRO	B	147	44.461	-7.892	75.871	1.00	17.58
ATOM	4169	N	ALA	B	148	43.568	-7.172	77.809	1.00	15.81
ATOM	4170	CA	ALA	B	148	42.732	-8.362	78.008	1.00	19.82
ATOM	4171	CB	ALA	B	148	42.049	-8.312	79.372	1.00	17.50
ATOM	4172	C	ALA	B	148	41.683	-8.473	76.903	1.00	22.58
ATOM	4173	O	ALA	B	148	41.419	-9.567	76.404	1.00	18.38
ATOM	4174	N	VAL	B	149	41.080	-7.341	76.540	1.00	22.48
ATOM	4175	CA	VAL	B	149	40.086	-7.300	75.466	1.00	19.04
ATOM	4176	CB	VAL	B	149	39.503	-5.877	75.281	1.00	18.96
ATOM	4177	CG1	VAL	B	149	38.691	-5.800	73.988	1.00	17.32
ATOM	4178	CG2	VAL	B	149	38.621	-5.531	76.462	1.00	15.33
ATOM	4179	C	VAL	B	149	40.763	-7.709	74.166	1.00	22.12
ATOM	4180	O	VAL	B	149	40.240	-8.535	73.421	1.00	21.83
ATOM	4181	N	GLY	B	150	41.927	-7.120	73.903	1.00	19.51

ATOM	4182	CA	GLY	B	150	42.657	-7.433	72.689	1.00	19.32
ATOM	4183	C	GLY	B	150	43.033	-8.901	72.606	1.00	19.59
ATOM	4184	O	GLY	B	150	42.962	-9.550	71.568	1.00	22.28
ATOM	4185	N	ILE	B	151	43.558	-9.435	73.700	1.00	19.51
ATOM	4186	CA	ILE	B	151	43.958	-10.834	73.723	1.00	23.21
ATOM	4187	CB	ILE	B	151	44.666	-11.175	75.053	1.00	23.50
ATOM	4188	CG2	ILE	B	151	44.918	-12.679	75.158	1.00	20.01
ATOM	4189	CG1	ILE	B	151	45.988	-10.394	75.129	1.00	21.98
ATOM	4190	CD1	ILE	B	151	46.716	-10.502	76.457	1.00	21.24
ATOM	4191	C	ILE	B	151	42.749	-11.741	73.490	1.00	28.40
ATOM	4192	O	ILE	B	151	42.832	-12.692	72.706	1.00	22.96
ATOM	4193	N	GLU	B	152	41.623	-11.450	74.144	1.00	27.32
ATOM	4194	CA	GLU	B	152	40.417	-12.265	73.939	1.00	27.62
ATOM	4195	CB	GLU	B	152	39.294	-11.845	74.886	1.00	26.46
ATOM	4196	CG	GLU	B	152	39.533	-12.200	76.347	1.00	28.26
ATOM	4197	CD	GLU	B	152	39.613	-13.708	76.592	1.00	31.10
ATOM	4198	OE1	GLU	B	152	39.668	-14.123	77.767	1.00	29.55
ATOM	4199	OE2	GLU	B	152	39.626	-14.481	75.617	1.00	30.51
ATOM	4200	C	GLU	B	152	39.948	-12.125	72.497	1.00	30.30
ATOM	4201	O	GLU	B	152	39.463	-13.082	71.893	1.00	25.58
ATOM	4202	N	TYR	B	153	40.093	-10.923	71.948	1.00	26.23
ATOM	4203	CA	TYR	B	153	39.720	-10.669	70.563	1.00	28.19
ATOM	4204	CB	TYR	B	153	40.082	-9.235	70.190	1.00	27.94
ATOM	4205	CG	TYR	B	153	39.379	-8.886	68.735	1.00	28.46
ATOM	4206	CD1	TYR	B	153	38.618	-8.560	68.240	1.00	25.69
ATOM	4207	CE1	TYR	B	153	38.447	-8.195	66.898	1.00	30.73
ATOM	4208	CD2	TYR	B	153	40.962	-8.847	67.856	1.00	24.82
ATOM	4209	CE2	TYR	B	153	40.801	-8.488	66.526	1.00	29.26
ATOM	4210	CZ	TYR	B	153	39.547	-8.161	66.054	1.00	31.25
ATOM	4211	OH	TYR	B	153	39.406	-7.803	64.735	1.00	34.22
ATOM	4212	C	TYR	B	153	40.513	-11.627	69.674	1.00	28.11
ATOM	4213	O	TYR	B	153	39.975	-12.248	68.759	1.00	22.06
ATOM	4214	N	LEU	B	154	41.810	-11.725	69.944	1.00	26.77
ATOM	4215	CA	LEU	B	154	42.681	-12.597	69.168	1.00	28.79
ATOM	4216	CB	LEU	B	154	44.142	-12.386	69.592	1.00	28.06
ATOM	4217	CG	LEU	B	154	44.789	-11.087	69.083	1.00	27.71
ATOM	4218	CD1	LEU	B	154	46.119	-10.860	69.759	1.00	34.15
ATOM	4219	CD2	LEU	B	154	44.968	-11.171	67.571	1.00	26.71
ATOM	4220	C	LEU	B	154	42.299	-14.074	69.274	1.00	26.98
ATOM	4221	O	LEU	B	154	42.282	-14.787	68.271	1.00	29.88
ATOM	4222	N	ARG	B	155	41.996	-14.536	70.480	1.00	23.19
ATOM	4223	CA	ARG	B	155	41.622	-15.936	70.669	1.00	29.47
ATOM	4224	CB	ARG	B	155	41.339	-16.230	72.144	1.00	28.53
ATOM	4225	CG	ARG	B	155	42.527	-15.965	73.053	1.00	35.03
ATOM	4226	CD	ARG	B	155	42.212	-16.276	74.507	1.00	39.42
ATOM	4227	NE	ARG	B	155	42.165	-17.706	74.792	1.00	30.99
ATOM	4228	CZ	ARG	B	155	41.869	-18.209	75.986	1.00	41.33
ATOM	4229	NH1	ARG	B	155	41.591	-17.394	77.002	1.00	38.47
ATOM	4230	NH2	ARG	B	155	41.872	-19.523	76.178	1.00	40.67
ATOM	4231	C	ARG	B	155	40.393	-16.260	69.832	1.00	29.07
ATOM	4232	O	ARG	B	155	40.325	-17.311	69.203	1.00	25.31
ATOM	4233	N	LYS	B	156	39.419	-15.357	69.828	1.00	28.99
ATOM	4234	CA	LYS	B	156	38.216	-15.573	69.038	1.00	34.63
ATOM	4235	CB	LYS	B	156	37.148	-14.534	69.386	1.00	36.63
ATOM	4236	CG	LYS	B	156	36.393	-14.883	70.646	1.00	42.18
ATOM	4237	CD	LYS	B	156	37.292	-14.900	71.868	1.00	51.38
ATOM	4238	CE	LYS	B	156	36.685	-15.712	73.009	1.00	52.76
ATOM	4239	NZ	LYS	B	156	36.661	-17.172	72.677	1.00	51.29
ATOM	4240	C	LYS	B	156	38.504	-15.562	67.538	1.00	34.66
ATOM	4241	O	LYS	B	156	37.722	-16.088	66.754	1.00	33.53
ATOM	4242	N	LYS	B	157	39.625	-14.966	67.140	1.00	30.06
ATOM	4243	CA	LYS	B	157	39.996	-14.945	65.734	1.00	31.26
ATOM	4244	CB	LYS	B	157	40.888	-13.746	65.418	1.00	29.79
ATOM	4245	CG	LYS	B	157	40.157	-12.426	65.359	1.00	31.52
ATOM	4246	CD	LYS	B	157	39.132	-12.424	64.239	1.00	28.48
ATOM	4247	CE	LYS	B	157	38.395	-11.101	64.171	1.00	31.90

Figure 18-65

ATOM	4248	NZ	LYS	B	157	37.406	-11.080	63.054	1.00	32.91
ATOM	4249	C	LYS	B	157	40.724	-16.234	65.381	1.00	31.92
ATOM	4250	O	LYS	B	157	41.146	-16.421	64.246	1.00	33.58
ATOM	4251	N	GLY	B	158	40.890	-17.111	66.368	1.00	28.97
ATOM	4252	CA	GLY	B	158	41.546	-18.379	66.112	1.00	28.98
ATOM	4253	C	GLY	B	158	42.962	-18.569	66.622	1.00	33.33
ATOM	4254	O	GLY	B	158	43.503	-19.672	66.522	1.00	30.58
ATOM	4255	N	PHE	B	159	43.578	-17.521	67.164	1.00	32.80
ATOM	4256	CA	PHE	B	159	44.937	-17.657	67.678	1.00	28.89
ATOM	4257	CB	PHE	B	159	45.560	-16.286	67.934	1.00	30.33
ATOM	4258	CG	PHE	B	159	45.748	-15.470	66.692	1.00	28.53
ATOM	4259	CD1	PHE	B	159	44.682	-14.787	66.121	1.00	24.58
ATOM	4260	CD2	PHE	B	159	46.989	-15.420	66.068	1.00	24.21
ATOM	4261	CE1	PHE	B	159	44.849	-14.066	64.948	1.00	25.26
ATOM	4262	CE2	PHE	B	159	47.168	-14.706	64.895	1.00	23.66
ATOM	4263	CZ	PHE	B	159	46.095	-14.026	64.332	1.00	26.65
ATOM	4264	C	PHE	B	159	44.969	-18.484	68.958	1.00	30.92
ATOM	4265	O	PHE	B	159	44.102	-18.334	69.820	1.00	24.26
ATOM	4266	N	LYS	B	160	45.979	-19.347	69.077	1.00	28.86
ATOM	4267	CA	LYS	B	160	46.123	-20.224	70.237	1.00	30.27
ATOM	4268	CB	LYS	B	160	46.085	-21.692	69.800	1.00	32.05
ATOM	4269	CG	LYS	B	160	44.806	-22.117	69.113	1.00	41.13
ATOM	4270	CD	LYS	B	160	44.809	-23.621	68.826	1.00	40.73
ATOM	4271	CE	LYS	B	160	45.945	-24.031	67.904	1.00	43.16
ATOM	4272	NZ	LYS	B	160	45.812	-23.408	66.554	1.00	48.69
ATOM	4273	C	LYS	B	160	47.394	-19.997	71.048	1.00	28.23
ATOM	4274	O	LYS	B	160	47.552	-20.561	72.130	1.00	25.29
ATOM	4275	N	ARG	B	161	48.320	-19.206	70.520	1.00	28.51
ATOM	4276	CA	ARG	B	161	49.550	-18.921	71.247	1.00	25.84
ATOM	4277	CB	ARG	B	161	50.724	-19.719	70.667	1.00	25.33
ATOM	4278	CG	ARG	B	161	50.551	-21.245	70.781	1.00	27.47
ATOM	4279	CD	ARG	B	161	51.833	-21.985	70.394	1.00	32.27
ATOM	4280	NE	ARG	B	161	52.218	-21.761	69.002	1.00	34.90
ATOM	4281	CZ	ARG	B	161	51.584	-22.276	67.954	1.00	38.45
ATOM	4282	NH1	ARG	B	161	50.527	-23.056	68.130	1.00	38.77
ATOM	4283	NH2	ARG	B	161	51.999	-22.000	66.725	1.00	38.64
ATOM	4284	C	ARG	B	161	49.818	-17.421	71.182	1.00	30.40
ATOM	4285	O	ARG	B	161	50.393	-16.912	70.218	1.00	27.50
ATOM	4286	N	ILE	B	162	49.376	-16.722	72.221	1.00	25.64
ATOM	4287	CA	ILE	B	162	49.515	-15.273	72.303	1.00	27.44
ATOM	4288	CB	ILE	B	162	48.134	-14.618	72.545	1.00	24.53
ATOM	4289	CG2	ILE	B	162	48.249	-13.101	72.473	1.00	25.49
ATOM	4290	CG1	ILE	B	162	47.142	-15.101	71.487	1.00	29.46
ATOM	4291	CD1	ILE	B	162	45.688	-14.707	71.758	1.00	31.94
ATOM	4292	C	ILE	B	162	50.465	-14.868	73.429	1.00	22.68
ATOM	4293	O	ILE	B	162	52.311	-15.302	74.568	1.00	24.25
ATOM	4294	N	LEU	B	163	52.454	-14.042	73.100	1.00	19.49
ATOM	4295	CA	LEU	B	163	52.425	-13.561	74.081	1.00	17.57
ATOM	4296	CB	LEU	B	163	53.850	-13.686	73.528	1.00	20.54
ATOM	4297	CG	LEU	B	163	54.979	-12.975	74.295	1.00	18.84
ATOM	4298	CD1	LEU	B	163	55.102	-13.538	75.690	1.00	20.55
ATOM	4299	CD2	LEU	B	163	56.293	-13.148	73.556	1.00	18.57
ATOM	4300	C	LEU	B	163	52.158	-12.099	74.430	1.00	16.20
ATOM	4301	O	LEU	B	163	51.898	-11.277	73.549	1.00	16.09
ATOM	4302	N	TYR	B	164	52.227	-11.780	75.715	1.00	14.05
ATOM	4303	CA	TYR	B	164	52.027	-10.411	76.191	1.00	16.21
ATOM	4304	CB	TYR	B	164	50.777	-10.323	77.070	1.00	16.01
ATOM	4305	CG	TYR	B	164	50.534	-8.948	77.667	1.00	15.08
ATOM	4306	CD1	TYR	B	164	50.148	-7.869	76.869	1.00	19.51
ATOM	4307	CE1	TYR	B	164	49.948	-6.597	77.418	1.00	12.88
ATOM	4308	CD2	TYR	B	164	50.715	-8.724	79.021	1.00	14.07
ATOM	4309	CE2	TYR	B	164	50.520	-7.463	79.583	1.00	13.66
ATOM	4310	CZ	TYR	B	164	50.139	-6.407	78.782	1.00	14.72
ATOM	4311	OH	TYR	B	164	49.952	-5.163	79.354	1.00	13.54
ATOM	4312	C	TYR	B	164	53.246	-10.017	77.018	1.00	19.14
ATOM	4313	O	TYR	B	164	53.539	-10.642	78.036	1.00	26.51

ATOM	4314	N	ILE	B	165	53.964	-8.992	76.573	1.00	22.40
ATOM	4315	CA	ILE	B	165	55.148	-8.518	77.285	1.00	17.72
ATOM	4316	CB	ILE	B	165	56.352	-8.465	76.343	1.00	22.51
ATOM	4317	CG2	ILE	B	165	57.582	-7.902	77.079	1.00	16.36
ATOM	4318	CG1	ILE	B	165	56.632	-9.880	75.818	1.00	19.82
ATOM	4319	CD1	ILE	B	165	57.721	-9.942	74.742	1.00	21.74
ATOM	4320	C	ILE	B	165	54.851	-7.126	77.850	1.00	22.54
ATOM	4321	O	ILE	B	165	54.478	-6.223	77.111	1.00	16.60
ATOM	4322	N	ASP	B	166	55.046	-6.961	79.156	1.00	15.78
ATOM	4323	CA	ASP	B	166	54.740	-5.704	79.840	1.00	20.62
ATOM	4324	CB	ASP	B	166	53.719	-5.996	80.949	1.00	17.57
ATOM	4325	CG	ASP	B	166	53.063	-4.742	81.486	1.00	25.39
ATOM	4326	OD1	ASP	B	166	53.779	-3.859	82.003	1.00	19.68
ATOM	4327	OD2	ASP	B	166	51.824	-4.637	81.377	1.00	29.22
ATOM	4328	C	ASP	B	166	55.976	-5.002	80.423	1.00	19.01
ATOM	4329	O	ASP	B	166	56.509	-5.412	81.456	1.00	19.74
ATOM	4330	N	LEU	B	167	56.414	-3.923	79.775	1.00	17.88
ATOM	4331	CA	LEU	B	167	57.598	-3.211	80.235	1.00	14.99
ATOM	4332	CB	LEU	B	167	58.412	-2.710	79.044	1.00	19.22
ATOM	4333	CG	LEU	B	167	58.871	-3.799	78.069	1.00	22.68
ATOM	4334	CD1	LEU	B	167	59.835	-3.179	77.074	1.00	25.35
ATOM	4335	CD2	LEU	B	167	59.570	-4.943	78.808	1.00	17.54
ATOM	4336	C	LEU	B	167	57.284	-2.059	81.183	1.00	17.49
ATOM	4337	O	LEU	B	167	58.189	-1.359	81.639	1.00	13.39
ATOM	4338	N	ASP	S	168	56.003	-1.878	81.479	1.00	20.03
ATOM	4339	CA	ASP	B	168	55.549	-0.848	82.412	1.00	21.98
ATOM	4340	CB	ASP	B	168	54.030	-0.955	82.597	1.00	21.21
ATOM	4341	CG	ASP	B	168	53.453	0.186	83.428	1.00	24.92
ATOM	4342	C	ASP	B	168	56.241	-1.139	83.753	1.00	22.98
ATOM	4343	O	ASP	B	168	56.447	-2.304	84.091	1.00	18.36
ATOM	4344	OD1	ASP	B	168	52.849	1.099	82.825	1.00	22.03
ATOM	4345	OD2	ASP	B	168	53.606	0.189	84.676	1.00	18.43
ATOM	4346	N	ALA	B	169	56.581	-0.095	84.514	1.00	15.46
ATOM	4347	CA	ALA	B	169	57.263	-0.268	85.807	1.00	18.73
ATOM	4348	CB	ALA	B	169	57.764	1.084	86.323	1.00	11.98
ATOM	4349	C	ALA	B	169	56.400	-0.940	86.886	1.00	21.82
ATOM	4350	O	ALA	B	169	56.886	-1.262	87.980	1.00	22.51
ATOM	4351	N	HIS	B	170	55.120	-1.134	86.600	1.00	18.75
ATOM	4352	CA	HIS	B	170	54.238	-1.776	87.570	1.00	22.70
ATOM	4353	C	HIS	B	170	53.716	-3.096	87.015	1.00	22.11
ATOM	4354	O	HIS	B	170	53.536	-3.244	85.809	1.00	21.94
ATOM	4355	CB	HIS	B	170	53.050	-0.867	87.927	1.00	21.28
ATOM	4356	CG	HIS	B	170	53.449	0.475	88.460	1.00	18.89
ATOM	4357	ND1	HIS	B	170	53.695	1.539	87.626	1.00	19.13
ATOM	4358	CE1	HIS	B	170	54.046	2.539	88.412	1.00	19.41
ATOM	4359	CD2	HIS	B	170	53.660	0.854	89.746	1.00	19.02
ATOM	4360	NE2	HIS	B	170	54.042	2.174	89.710	1.00	20.45
ATOM	4361	N	HIS	B	171	53.474	-4.047	87.907	1.00	19.20
ATOM	4362	CA	HIS	B	171	52.961	-5.352	87.519	1.00	21.20
ATOM	4363	CB	HIS	B	171	52.964	-6.284	88.722	1.00	22.00
ATOM	4364	CG	HIS	B	171	52.541	-7.683	88.400	1.00	24.64
ATOM	4365	CD2	HIS	B	171	53.056	-8.594	87.540	1.00	19.19
ATOM	4366	ND1	HIS	B	171	51.441	-8.279	88.979	1.00	25.71
ATOM	4367	CE1	HIS	B	171	51.295	-9.497	88.487	1.00	25.30
ATOM	4368	NE2	HIS	B	171	52.261	-9.713	87.612	1.00	24.71
ATOM	4369	C	HIS	B	171	51.549	-5.306	86.943	1.00	23.91
ATOM	4370	O	HIS	B	171	50.677	-4.620	87.479	1.00	18.93
ATOM	4371	N	CYS	B	172	51.332	-6.062	85.865	1.00	15.36
ATOM	4372	CA	CYS	B	172	50.036	-6.141	85.207	1.00	20.03
ATOM	4373	CB	CYS	B	172	50.240	-6.534	83.732	1.00	22.46
ATOM	4374	SG	CYS	B	172	51.259	-3.030	83.419	1.00	23.49
ATOM	4375	C	CYS	B	172	49.110	-7.146	85.913	1.00	18.05
ATOM	4376	O	CYS	B	172	48.712	-8.151	85.327	1.00	18.23
ATOM	4377	N	ASP	B	173	48.767	-6.871	87.170	1.00	16.78
ATOM	4378	CA	ASP	B	173	47.909	-7.776	87.928	1.00	18.81
ATOM	4379	CB	ASP	B	173	47.638	-7.236	89.344	1.00	20.39

Figure 18-67

ATOM	4380	CG	ASP	B	173	46.961	-5.871	89.354	1.00	23.40
ATOM	4381	OD1	ASP	B	173	46.564	-5.435	90.455	1.00	18.64
ATOM	4382	OD2	ASP	B	173	46.834	-5.231	88.291	1.00	19.24
ATOM	4383	C	ASP	B	173	46.595	-8.116	87.219	1.00	17.46
ATOM	4384	O	ASP	B	173	46.162	-9.272	87.224	1.00	15.53
ATOM	4385	N	GLY	B	174	45.978	-7.130	86.580	1.00	13.46
ATOM	4386	CA	GLY	B	174	44.733	-7.391	85.876	1.00	18.18
ATOM	4387	C	GLY	B	174	44.904	-8.392	84.741	1.00	17.85
ATOM	4388	O	GLY	B	174	44.104	-9.316	84.583	1.00	18.27
ATOM	4389	N	VAL	B	175	45.951	-8.214	83.943	1.00	16.14
ATOM	4390	CA	VAL	B	175	46.206	-9.111	82.829	1.00	17.00
ATOM	4391	CB	VAL	B	175	47.305	-8.552	81.902	1.00	27.22
ATOM	4392	CG1	VAL	B	175	47.533	-9.507	80.731	1.00	19.75
ATOM	4393	CG2	VAL	B	175	46.896	-7.169	81.396	1.00	18.66
ATOM	4394	C	VAL	B	175	46.635	-10.486	83.324	1.00	22.82
ATOM	4395	O	VAL	B	175	46.255	-11.503	82.754	1.00	18.06
ATOM	4396	N	GLN	B	176	47.439	-10.520	84.378	1.00	21.67
ATOM	4397	CA	GLN	B	176	47.889	-11.798	84.911	1.00	21.55
ATOM	4398	CB	GLN	B	176	48.824	-11.602	86.105	1.00	19.68
ATOM	4399	CG	GLN	B	176	49.088	-12.905	86.862	1.00	20.17
ATOM	4400	CD	GLN	B	176	50.066	-12.759	87.996	1.00	25.42
ATOM	4401	OE1	GLN	B	176	51.243	-12.442	87.786	1.00	21.56
ATOM	4402	NE2	GLN	B	176	49.592	-13.000	89.217	1.00	20.18
ATOM	4403	C	GLN	B	176	46.689	-12.630	85.348	1.00	24.78
ATOM	4404	O	GLN	B	176	46.618	-13.817	85.057	1.00	22.91
ATOM	4405	N	GLU	B	177	45.751	-12.007	86.051	1.00	23.69
ATOM	4406	CA	GLU	B	177	44.571	-12.727	86.523	1.00	27.01
ATOM	4407	CB	GLU	B	177	43.703	-11.825	87.394	1.00	24.73
ATOM	4408	CG	GLU	B	177	42.633	-12.581	88.138	1.00	37.46
ATOM	4409	CD	GLU	B	177	41.767	-11.676	88.987	1.00	42.48
ATOM	4410	OE1	GLU	B	177	40.875	-11.002	88.432	1.00	44.35
ATOM	4411	OE2	GLU	B	177	41.993	-11.627	90.213	1.00	45.63
ATOM	4412	C	GLU	B	177	43.732	-13.247	85.370	1.00	26.56
ATOM	4413	O	GLU	B	177	43.240	-14.375	85.408	1.00	27.71
ATOM	4414	N	ALA	B	178	43.573	-12.418	84.344	1.00	24.58
ATOM	4415	CA	ALA	B	178	42.776	-12.775	83.174	1.00	25.86
ATOM	4416	CB	ALA	B	178	42.778	-11.628	82.171	1.00	24.20
ATOM	4417	C	ALA	B	178	43.231	-14.054	82.485	1.00	25.72
ATOM	4418	O	ALA	B	178	42.406	-14.838	82.036	1.00	22.38
ATOM	4419	N	PHE	B	179	44.535	-14.282	82.395	1.00	27.19
ATOM	4420	CA	PHE	B	179	44.990	-15.489	81.703	1.00	27.05
ATOM	4421	CB	PHE	B	179	45.714	-15.086	80.418	1.00	25.22
ATOM	4422	CG	PHE	B	179	44.992	-14.020	79.644	1.00	20.36
ATOM	4423	CD1	PHE	B	179	45.387	-12.687	79.735	1.00	25.23
ATOM	4424	CD2	PHE	B	179	43.860	-14.332	78.902	1.00	19.22
ATOM	4425	CE1	PHE	B	179	44.659	-11.677	79.102	1.00	19.25
ATOM	4426	CE2	PHE	B	179	43.128	-13.315	78.272	1.00	20.65
ATOM	4427	CZ	PHE	B	179	43.528	-12.001	78.374	1.00	25.64
ATOM	4428	C	PHE	B	179	45.866	-16.398	82.556	1.00	23.50
ATOM	4429	O	PHE	B	179	46.652	-17.182	82.038	1.00	18.26
ATOM	4430	N	TYR	B	180	45.689	-16.313	83.868	1.00	23.24
ATOM	4431	CA	TYR	B	180	46.479	-17.106	84.799	1.00	26.76
ATOM	4432	CB	TYR	B	180	46.150	-16.665	86.231	1.00	25.72
ATOM	4433	CG	TYR	B	180	47.226	-16.969	87.247	1.00	29.66
ATOM	4434	CD1	TYR	B	180	47.037	-17.942	88.237	1.00	27.07
ATOM	4435	CE1	TYR	B	180	48.039	-18.222	89.170	1.00	30.08
ATOM	4436	CD2	TYR	B	180	48.444	-16.283	87.216	1.00	29.68
ATOM	4437	CE2	TYR	B	180	49.451	-16.552	88.139	1.00	30.99
ATOM	4438	CZ	TYR	B	180	49.248	-17.521	89.112	1.00	33.16
ATOM	4439	OH	TYR	B	180	50.262	-17.791	90.006	1.00	28.47
ATOM	4440	C	TYR	B	180	46.256	-18.619	84.649	1.00	29.13
ATOM	4441	O	TYR	B	180	47.163	-19.416	84.922	1.00	23.43
ATOM	4442	N	ASP	B	181	45.073	-19.021	84.190	1.00	25.67
ATOM	4443	CA	ASP	B	181	44.784	-20.445	84.075	1.00	28.28
ATOM	4444	CB	ASP	B	181	43.446	-20.759	84.757	1.00	32.13
ATOM	4445	CG	ASP	B	181	42.247	-20.410	83.890	1.00	36.12

ATOM	4446	OD1	ASP	B	181	42.202	-19.300	83.329	1.00	41.04
ATOM	4447	OD2	ASP	B	181	41.334	-21.249	83.782	1.00	44.36
ATOM	4448	C	ASP	B	181	44.773	-21.018	82.664	1.00	32.41
ATOM	4449	O	ASP	B	181	44.246	-22.115	82.444	1.00	31.67
ATOM	4450	N	THR	B	182	45.345	-20.302	81.702	1.00	29.24
ATOM	4451	CA	THR	B	182	45.363	-20.823	80.340	1.00	30.57
ATOM	4452	CB	THR	B	182	44.468	-20.008	79.397	1.00	30.03
ATOM	4453	OG1	THR	B	182	44.516	-20.598	78.095	1.00	28.22
ATOM	4454	CG2	THR	B	182	44.947	-18.561	79.310	1.00	26.55
ATOM	4455	C	THR	B	182	46.759	-20.870	79.740	1.00	32.31
ATOM	4456	O	THR	B	182	47.591	-20.007	80.008	1.00	27.27
ATOM	4457	N	ASP	B	183	46.999	-21.878	78.909	1.00	29.94
ATOM	4458	CA	ASP	B	183	48.296	-22.049	78.273	1.00	31.40
ATOM	4459	CB	ASP	B	183	48.648	-23.536	78.228	1.00	33.36
ATOM	4460	CG	ASP	B	183	47.718	-24.319	77.328	1.00	33.33
ATOM	4461	OD1	ASP	B	183	46.513	-23.988	77.287	1.00	28.06
ATOM	4462	OD2	ASP	B	183	48.186	-25.271	76.675	1.00	38.19
ATOM	4463	C	ASP	B	183	48.321	-21.462	76.864	1.00	31.14
ATOM	4464	O	ASP	B	183	49.332	-21.557	76.168	1.00	28.74
ATOM	4465	N	GLN	B	184	47.217	-20.852	76.446	1.00	25.34
ATOM	4466	CA	GLN	B	184	47.151	-20.251	75.118	1.00	28.59
ATOM	4467	CB	GLN	B	184	45.712	-20.256	74.581	1.00	26.84
ATOM	4468	CG	GLN	B	184	45.060	-21.632	74.529	1.00	34.86
ATOM	4469	CD	GLN	B	184	43.760	-21.647	73.736	1.00	32.27
ATOM	4470	OE1	GLN	B	184	42.897	-20.789	73.912	1.00	35.43
ATOM	4471	NE2	GLN	B	184	43.611	-22.641	72.870	1.00	28.92
ATOM	4472	C	GLN	B	184	47.672	-18.817	75.175	1.00	27.28
ATOM	4473	O	GLN	B	184	47.871	-18.171	74.148	1.00	29.70
ATOM	4474	N	VAL	B	185	47.900	-18.325	76.386	1.00	27.64
ATOM	4475	CA	VAL	B	185	48.400	-16.972	76.575	1.00	26.26
ATOM	4476	CB	VAL	B	185	47.304	-16.039	77.145	1.00	22.85
ATOM	4477	CG1	VAL	B	185	47.879	-14.642	77.395	1.00	23.10
ATOM	4478	CG2	VAL	B	185	46.136	-15.967	76.191	1.00	21.67
ATOM	4479	C	VAL	B	185	49.570	-16.964	77.547	1.00	27.01
ATOM	4480	O	VAL	B	185	49.456	-17.469	78.663	1.00	23.75
ATOM	4481	N	PHE	B	186	50.696	-16.403	77.115	1.00	22.02
ATOM	4482	CA	PHE	B	186	51.868	-16.301	77.978	1.00	21.83
ATOM	4483	CB	PHE	B	186	53.142	-16.763	77.252	1.00	17.02
ATOM	4484	CG	PHE	B	186	54.336	-16.921	78.170	1.00	24.84
ATOM	4485	CD1	PHE	B	186	54.756	-18.189	78.580	1.00	22.70
ATOM	4486	CD2	PHE	B	186	55.004	-15.805	78.670	1.00	20.26
ATOM	4487	CE1	PHE	B	186	55.819	-18.338	79.471	1.00	21.47
ATOM	4488	CE2	PHE	B	186	56.071	-15.941	79.563	1.00	20.01
ATOM	4489	CZ	PHE	B	186	56.481	-17.206	79.968	1.00	17.84
ATOM	4490	C	PHE	B	186	52.032	-14.827	78.368	1.00	18.12
ATOM	4491	O	PHE	B	186	52.038	-13.946	77.508	1.00	15.92
ATOM	4492	N	VAL	B	187	52.161	-14.565	79.661	1.00	18.06
ATOM	4493	CA	VAL	B	187	52.348	-13.208	80.153	1.00	17.67
ATOM	4494	CB	VAL	B	187	51.282	-12.839	81.225	1.00	22.85
ATOM	4495	CG1	VAL	B	187	51.608	-11.473	81.840	1.00	24.08
ATOM	4496	CG2	VAL	B	187	49.882	-12.808	80.598	1.00	18.82
ATOM	4497	C	VAL	B	187	53.735	-13.060	80.788	1.00	18.32
ATOM	4498	O	VAL	B	187	54.092	-13.807	81.707	1.00	18.82
ATOM	4499	N	LEU	B	188	54.503	-12.103	80.282	1.00	14.70
ATOM	4500	CA	LEU	B	188	55.832	-11.789	80.798	1.00	18.84
ATOM	4501	CB	LEU	B	188	56.900	-11.948	79.716	1.00	18.64
ATOM	4502	CG	LEU	B	188	58.230	-11.277	80.082	1.00	21.23
ATOM	4503	CD1	LEU	B	188	58.769	-11.832	81.395	1.00	18.55
ATOM	4504	CD2	LEU	B	188	59.227	-11.489	78.957	1.00	20.49
ATOM	4505	C	LEU	B	188	55.836	-10.339	81.280	1.00	22.14
ATOM	4506	O	LEU	B	188	55.527	-9.410	80.517	1.00	19.96
ATOM	4507	N	SER	B	189	56.187	-10.133	82.540	1.00	21.08
ATOM	4508	CA	SER	B	189	56.203	-8.782	83.061	1.00	21.85
ATOM	4509	CB	SER	B	189	54.956	-8.543	83.908	1.00	25.95
ATOM	4510	OG	SER	B	189	54.988	-7.252	84.475	1.00	21.91
ATOM	4511	C	SER	B	189	57.423	-8.420	83.883	1.00	23.62

ATOM	4512	O	SER	B	189	57.829	-9.174	84.766	1.00	18.61
ATOM	4513	N	LEU	B	190	58.020	-7.269	83.569	1.00	20.33
ATOM	4514	CA	LEU	B	190	59.149	-6.767	84.347	1.00	21.85
ATOM	4515	CB	LEU	B	190	60.278	-6.226	83.473	1.00	22.85
ATOM	4516	CG	LEU	B	190	60.964	-7.089	82.413	1.00	32.59
ATOM	4517	CD1	LEU	B	190	62.337	-6.479	82.140	1.00	29.27
ATOM	4518	CD2	LEU	B	190	61.136	-8.511	82.879	1.00	31.98
ATOM	4519	C	LEU	B	190	58.505	-5.613	85.085	1.00	21.28
ATOM	4520	O	LEU	B	190	57.695	-4.897	84.501	1.00	15.72
ATOM	4521	N	HIS	B	191	58.857	-5.421	86.351	1.00	18.16
ATOM	4522	CA	HIS	B	191	58.249	-4.357	87.145	1.00	17.46
ATOM	4523	CB	HIS	B	191	56.759	-4.690	87.369	1.00	16.00
ATOM	4524	CG	HIS	B	191	56.517	-6.085	87.880	1.00	22.14
ATOM	4525	CD2	HIS	B	191	56.341	-6.551	89.143	1.00	12.25
ATOM	4526	ND1	HIS	B	191	56.372	-7.179	87.049	1.00	18.02
ATOM	4527	CE1	HIS	B	191	56.119	-8.256	87.775	1.00	8.17
ATOM	4528	NE2	HIS	B	191	56.094	-7.902	89.049	1.00	19.79
ATOM	4529	C	HIS	B	191	58.945	-4.197	88.484	1.00	17.41
ATOM	4530	O	HIS	B	191	59.769	-5.029	88.867	1.00	18.74
ATOM	4531	N	GLN	B	192	58.618	-3.114	89.182	1.00	18.20
ATOM	4532	CA	GLN	B	192	59.173	-2.854	90.502	1.00	18.41
ATOM	4533	CB	GLN	B	192	58.690	-1.500	91.034	1.00	20.71
ATOM	4534	CG	GLN	B	192	58.871	-0.334	90.072	1.00	21.49
ATOM	4535	CD	GLN	B	192	58.226	0.930	90.594	1.00	20.65
ATOM	4536	OE1	GLN	B	192	58.775	1.615	91.459	1.00	21.52
ATOM	4537	NE2	GLN	B	192	57.029	1.226	90.098	1.00	15.10
ATOM	4538	C	GLN	B	192	58.608	-3.945	91.395	1.00	17.55
ATOM	4539	O	GLN	B	192	57.415	-4.256	91.320	1.00	17.48
ATOM	4540	N	SER	B	193	59.447	-4.522	92.240	1.00	15.71
ATOM	4541	CA	SER	B	193	58.986	-5.574	93.143	1.00	20.58
ATOM	4542	CB	SER	B	193	60.093	-5.963	94.120	1.00	20.71
ATOM	4543	OG	SER	B	193	59.571	-6.804	95.138	1.00	22.55
ATOM	4544	C	SER	B	193	57.774	-5.112	93.947	1.00	21.81
ATOM	4545	O	SER	B	193	57.769	-4.003	94.486	1.00	20.82
ATOM	4546	N	PRO	B	194	56.745	-5.967	94.063	1.00	21.80
ATOM	4547	CD	PRO	B	194	56.648	-7.331	93.524	1.00	24.27
ATOM	4548	CA	PRO	B	194	55.524	-5.643	94.812	1.00	23.58
ATOM	4549	CB	PRO	B	194	54.678	-6.909	94.642	1.00	22.98
ATOM	4550	CG	PRO	B	194	55.168	-7.458	93.317	1.00	26.35
ATOM	4551	C	PRO	B	194	55.841	-5.366	96.283	1.00	25.79
ATOM	4552	O	PRO	B	194	55.009	-4.831	97.022	1.00	27.26
ATOM	4553	N	GLU	B	195	57.045	-5.736	96.710	1.00	23.20
ATOM	4554	CA	GLU	B	195	57.428	-5.514	98.093	1.00	29.56
ATOM	4555	CB	GLU	B	195	58.816	-6.090	98.379	1.00	32.38
ATOM	4556	CG	GLU	B	195	58.940	-7.567	98.049	1.00	45.25
ATOM	4557	CD	GLU	B	195	60.206	-8.189	98.613	1.00	50.44
ATOM	4558	OE1	GLU	B	195	61.290	-7.580	98.471	1.00	50.51
ATOM	4559	OE2	GLU	B	195	60.118	-9.297	99.184	1.00	49.77
ATOM	4560	C	GLU	B	195	57.414	-4.035	98.425	1.00	25.11
ATOM	4561	O	GLU	B	195	57.095	-3.659	99.551	1.00	29.05
ATOM	4562	N	TYR	B	196	57.729	-3.191	97.445	1.00	22.90
ATOM	4563	CA	TYR	B	196	57.743	-1.750	97.696	1.00	22.46
ATOM	4564	CB	TYR	B	196	59.188	-1.223	97.668	1.00	22.72
ATOM	4565	CG	TYR	B	196	59.855	-1.234	96.301	1.00	24.17
ATOM	4566	CD1	TYR	B	196	59.639	-0.203	95.385	1.00	20.87
ATOM	4567	CE1	TYR	B	196	60.229	-0.222	94.118	1.00	18.31
ATOM	4568	CD2	TYR	B	196	60.684	-2.289	95.916	1.00	24.63
ATOM	4569	CE2	TYR	B	196	61.276	-2.318	94.648	1.00	24.39
ATOM	4570	CE	TYR	B	196	61.042	-1.284	93.756	1.00	23.01
ATOM	4571	OH	TYR	B	196	61.592	-1.328	92.492	1.00	19.86
ATOM	4572	C	TYR	B	196	56.896	-0.938	96.725	1.00	23.54
ATOM	4573	O	TYR	B	196	56.779	0.275	96.869	1.00	17.53
ATOM	4574	N	ALA	B	197	56.293	-1.589	95.740	1.00	22.11
ATOM	4575	CA	ALA	B	197	55.503	-0.829	94.779	1.00	24.28
ATOM	4576	CB	ALA	B	197	56.310	-0.616	93.513	1.00	23.03
ATOM	4577	C	ALA	B	197	54.153	-1.412	94.413	1.00	22.80

Figure 18-70

ATOM	4578	O	ALA	B	197	53.910	-2.609	94.549	1.00	17.67
ATOM	4579	N	PHE	B	198	53.278	-0.541	93.932	1.00	26.40
ATOM	4580	CA	PHE	B	198	51.956	-0.950	93.495	1.00	28.19
ATOM	4581	CB	PHE	B	198	51.152	0.263	93.035	1.00	29.51
ATOM	4582	CG	PHE	B	198	49.721	-0.050	92.711	1.00	29.50
ATOM	4583	CD1	PHE	B	198	48.732	0.100	93.674	1.00	32.77
ATOM	4584	CD2	PHE	B	198	49.367	-0.533	91.455	1.00	25.82
ATOM	4585	CE1	PHE	B	198	47.410	-0.223	93.394	1.00	36.70
ATOM	4586	CE2	PHE	B	198	48.050	-0.858	91.170	1.00	29.29
ATOM	4587	CZ	PHE	B	198	47.071	-0.703	92.141	1.00	33.05
ATOM	4588	C	PHE	B	198	52.170	-1.858	92.284	1.00	28.28
ATOM	4589	O	PHE	B	198	53.045	-1.602	91.456	1.00	27.15
ATOM	4590	N	PRO	B	199	51.407	-2.952	92.185	1.00	31.37
ATOM	4591	CD	PRO	B	199	51.440	-3.887	91.045	1.00	37.07
ATOM	4592	CA	PRO	B	199	50.386	-3.369	93.144	1.00	35.32
ATOM	4593	CB	PRO	B	199	49.545	-4.328	92.321	1.00	33.88
ATOM	4594	CG	PRO	B	199	50.641	-5.068	91.578	1.00	36.75
ATOM	4595	C	PRO	B	199	51.241	-4.082	94.184	1.00	36.93
ATOM	4596	O	PRO	B	199	52.308	-4.603	93.860	1.00	50.93
ATOM	4597	N	PHE	B	200	50.804	-4.127	95.422	1.00	37.04
ATOM	4598	CA	PHE	B	200	51.644	-4.763	96.421	1.00	30.13
ATOM	4599	CB	PHE	B	200	51.547	-3.968	97.723	1.00	28.70
ATOM	4600	CG	PHE	B	200	51.760	-2.485	97.543	1.00	29.98
ATOM	4601	CD1	PHE	B	200	50.717	-1.660	97.137	1.00	28.92
ATOM	4602	CD2	PHE	B	200	53.016	-1.919	97.746	1.00	23.60
ATOM	4603	CE1	PHE	B	200	50.922	-0.289	96.938	1.00	27.63
ATOM	4604	CE2	PHE	B	200	53.229	-0.558	97.547	1.00	23.56
ATOM	4605	CZ	PHE	B	200	52.182	0.260	97.143	1.00	28.37
ATOM	4606	C	PHE	B	200	51.296	-6.227	96.658	1.00	25.51
ATOM	4607	O	PHE	B	200	52.112	-6.984	97.167	1.00	20.92
ATOM	4608	N	GLU	B	201	50.094	-6.618	96.252	1.00	27.41
ATOM	4609	CA	GLU	B	201	49.576	-7.972	96.454	1.00	31.98
ATOM	4610	CB	GLU	B	201	48.056	-7.928	96.487	1.00	31.57
ATOM	4611	CG	GLU	B	201	47.486	-6.935	97.449	1.00	39.17
ATOM	4612	CD	GLU	B	201	45.987	-6.853	97.316	1.00	40.31
ATOM	4613	OE1	GLU	B	201	45.332	-7.902	97.500	1.00	38.90
ATOM	4614	OE2	GLU	B	201	45.475	-5.751	97.019	1.00	35.04
ATOM	4615	C	GLU	B	201	49.979	-9.018	95.422	1.00	30.83
ATOM	4616	O	GLU	B	201	49.901	-10.219	95.690	1.00	26.34
ATOM	4617	N	LYS	B	202	50.362	-8.573	94.234	1.00	24.95
ATOM	4618	CA	LYS	B	202	50.764	-9.501	93.195	1.00	22.79
ATOM	4619	CB	LYS	B	202	49.588	-9.773	92.258	1.00	25.12
ATOM	4620	CG	LYS	B	202	48.484	-10.523	93.000	1.00	35.38
ATOM	4621	CD	LYS	B	202	47.431	-11.099	92.103	1.00	38.67
ATOM	4622	CE	LYS	B	202	46.498	-11.998	92.903	1.00	40.98
ATOM	4623	NZ	LYS	B	202	45.491	-12.659	92.028	1.00	46.65
ATOM	4624	C	LYS	B	202	51.975	-9.007	92.435	1.00	24.62
ATOM	4625	O	LYS	B	202	52.355	-7.838	92.549	1.00	21.83
ATOM	4626	N	GLY	B	203	52.598	-9.910	91.684	1.00	17.60
ATOM	4627	CA	GLY	B	203	53.779	-9.545	90.928	1.00	19.41
ATOM	4628	C	GLY	B	203	55.014	-10.297	91.396	1.00	20.36
ATOM	4629	O	GLY	B	203	56.101	-10.070	90.888	1.00	23.83
ATOM	4630	N	PHE	B	204	54.855	-11.201	92.358	1.00	24.82
ATOM	4631	CA	PHE	B	204	55.992	-11.957	92.859	1.00	24.24
ATOM	4632	CB	PHE	B	204	55.690	-12.567	94.236	1.00	22.72
ATOM	4633	CG	PHE	B	204	55.485	-11.549	95.322	1.00	25.26
ATOM	4634	CD1	PHE	B	204	54.235	-10.977	95.535	1.00	23.80
ATOM	4635	CD2	PHE	B	204	56.551	-11.159	96.133	1.00	20.25
ATOM	4636	CE1	PHE	B	204	54.048	-10.036	96.545	1.00	29.98
ATOM	4637	CE2	PHE	B	204	56.377	-10.221	97.141	1.00	24.40
ATOM	4638	CZ	PHE	B	204	55.124	-9.658	97.350	1.00	25.54
ATOM	4639	C	PHE	B	204	56.412	-13.057	91.894	1.00	25.86
ATOM	4640	O	PHE	B	204	55.613	-13.540	91.091	1.00	20.65
ATOM	4641	N	LEU	B	205	57.676	-13.449	91.986	1.00	24.25
ATOM	4642	CA	LEU	B	205	58.233	-14.472	91.114	1.00	30.66
ATOM	4643	CB	LEU	B	205	59.723	-14.637	91.413	1.00	34.01

Figure 18-71

ATOM	4644	CG	LEU	B	205	60.495	-15.669	90.592	1.00	34.12
ATOM	4645	CD1	LEU	B	205	60.356	-15.382	89.109	1.00	32.95
ATOM	4646	CD2	LEU	B	205	61.957	-15.629	91.005	1.00	36.49
ATOM	4647	C	LEU	B	205	57.535	-15.827	91.205	1.00	30.51
ATOM	4648	O	LEU	B	205	57.467	-16.562	90.220	1.00	25.89
ATOM	4649	N	GLU	B	206	57.010	-16.147	92.382	1.00	30.43
ATOM	4650	CA	GLU	B	206	56.338	-17.423	92.605	1.00	30.64
ATOM	4651	CB	GLU	B	206	56.025	-17.601	94.093	1.00	34.77
ATOM	4652	CG	GLU	B	206	57.227	-17.512	95.033	1.00	42.50
ATOM	4653	CD	GLU	B	206	57.718	-16.084	95.270	1.00	45.76
ATOM	4654	OE1	GLU	B	206	58.228	-15.438	94.333	1.00	42.62
ATOM	4655	OE2	GLU	B	206	57.585	-15.602	96.413	1.00	50.22
ATOM	4656	C	GLU	B	206	55.045	-17.587	91.811	1.00	31.13
ATOM	4657	O	GLU	B	206	54.607	-18.708	91.563	1.00	28.18
ATOM	4658	N	GLU	B	207	54.430	-16.472	91.425	1.00	25.16
ATOM	4659	CA	GLU	B	207	53.178	-16.499	90.664	1.00	28.78
ATOM	4660	CB	GLU	B	207	52.546	-15.107	90.695	1.00	30.76
ATOM	4661	CG	GLU	B	207	52.121	-14.659	92.093	1.00	29.39
ATOM	4662	CD	GLU	B	207	52.057	-13.151	92.230	1.00	27.87
ATOM	4663	OE1	GLU	B	207	51.656	-12.477	91.261	1.00	24.38
ATOM	4664	OE2	GLU	B	207	52.389	-12.636	93.316	1.00	25.36
ATOM	4665	C	GLU	B	207	53.453	-16.922	89.224	1.00	29.48
ATOM	4666	O	GLU	B	207	53.658	-16.077	88.351	1.00	27.48
ATOM	4667	N	ILE	B	208	53.442	-18.230	88.976	1.00	26.67
ATOM	4668	CA	ILE	B	208	53.735	-18.754	87.646	1.00	32.60
ATOM	4669	CB	ILE	B	208	54.789	-19.877	87.740	1.00	34.26
ATOM	4670	CG2	ILE	B	208	55.239	-20.296	86.352	1.00	41.65
ATOM	4671	CG1	ILE	B	208	56.008	-19.404	88.532	1.00	36.07
ATOM	4672	CD1	ILE	B	208	56.814	-18.338	87.851	1.00	45.18
ATOM	4673	C	ILE	B	208	52.522	-19.289	86.870	1.00	32.26
ATOM	4674	O	ILE	B	208	52.668	-19.799	85.759	1.00	27.43
ATOM	4675	N	GLY	B	209	51.328	-19.165	87.442	1.00	32.60
ATOM	4676	CA	GLY	B	209	50.139	-19.652	86.760	1.00	35.07
ATOM	4677	C	GLY	B	209	49.565	-20.892	87.420	1.00	36.19
ATOM	4678	O	GLY	B	209	50.230	-21.524	88.235	1.00	31.61
ATOM	4679	N	GLU	B	210	48.335	-21.245	87.066	1.00	36.98
ATOM	4680	CA	GLU	B	210	47.677	-22.412	87.647	1.00	40.60
ATOM	4681	CB	GLU	B	210	46.633	-21.964	88.672	1.00	37.98
ATOM	4682	CG	GLU	B	210	45.446	-21.234	88.058	1.00	42.78
ATOM	4683	CD	GLU	B	210	44.470	-20.717	89.098	1.00	48.41
ATOM	4684	OE1	GLU	B	210	43.400	-20.202	88.709	1.00	51.03
ATOM	4685	OE2	GLU	B	210	44.778	-20.814	90.306	1.00	49.90
ATOM	4686	C	GLU	B	210	46.996	-23.248	86.564	1.00	39.48
ATOM	4687	O	GLU	B	210	46.709	-22.751	85.471	1.00	33.65
ATOM	4688	N	GLY	B	211	46.736	-24.515	86.876	1.00	39.18
ATOM	4689	CA	GLY	B	211	46.087	-25.399	85.923	1.00	38.43
ATOM	4690	C	GLY	B	211	46.877	-25.500	84.637	1.00	40.29
ATOM	4691	O	GLY	B	211	48.101	-25.610	84.666	1.00	39.39
ATOM	4692	N	LYS	B	212	46.187	-25.458	83.504	1.00	40.90
ATOM	4693	CA	LYS	B	212	46.864	-25.538	82.219	1.00	43.53
ATOM	4694	CB	LYS	B	212	45.842	-25.548	81.080	1.00	47.87
ATOM	4695	CG	LYS	B	212	44.795	-26.665	81.144	1.00	53.09
ATOM	4696	CD	LYS	B	212	45.398	-28.076	81.130	1.00	58.61
ATOM	4697	CE	LYS	B	212	46.069	-28.454	82.452	1.00	59.78
ATOM	4698	NZ	LYS	B	212	46.670	-29.825	82.420	1.00	62.17
ATOM	4699	C	LYS	B	212	47.823	-24.363	82.040	1.00	38.84
ATOM	4700	O	LYS	B	212	48.797	-24.457	81.295	1.00	40.33
ATOM	4701	N	GLY	B	213	47.543	-23.262	82.731	1.00	37.20
ATOM	4702	CA	GLY	B	213	48.384	-22.081	82.627	1.00	34.66
ATOM	4703	C	GLY	B	213	49.625	-22.107	83.505	1.00	37.09
ATOM	4704	O	GLY	B	213	50.425	-21.165	83.489	1.00	25.85
ATOM	4705	N	LYS	B	214	49.794	-23.180	84.273	1.00	33.33
ATOM	4706	CA	LYS	B	214	50.953	-23.297	85.148	1.00	37.90
ATOM	4707	CB	LYS	B	214	50.886	-24.598	85.954	1.00	38.89
ATOM	4708	CG	LYS	B	214	52.032	-24.786	86.938	1.00	39.29
ATOM	4709	CD	LYS	B	214	51.876	-26.094	87.704	1.00	43.60

Figure 18-72

ATOM	4710	CE	LYS	B	214	53.047	-26.334	88.640	1.00	47.36
ATOM	4711	NZ	LYS	B	214	53.165	-25.264	89.666	1.00	54.03
ATOM	4712	C	LYS	B	214	52.209	-23.275	84.291	1.00	34.16
ATOM	4713	O	LYS	B	214	52.404	-24.136	83.438	1.00	34.70
ATOM	4714	N	GLY	B	215	53.057	-22.279	84.523	1.00	33.58
ATOM	4715	CA	GLY	B	215	54.275	-22.152	83.743	1.00	28.27
ATOM	4716	C	GLY	B	215	54.104	-21.155	82.605	1.00	31.02
ATOM	4717	O	GLY	B	215	55.033	-20.911	81.833	1.00	23.68
ATOM	4718	N	TYR	B	216	52.918	-20.564	82.493	1.00	22.45
ATOM	4719	CA	TYR	B	216	52.683	-19.605	81.426	1.00	24.03
ATOM	4720	CB	TYR	B	216	51.458	-20.013	80.603	1.00	17.60
ATOM	4721	CG	TYR	B	216	51.682	-21.291	79.806	1.00	25.96
ATOM	4722	CD1	TYR	B	216	51.692	-22.538	80.435	1.00	21.41
ATOM	4723	CE1	TYR	B	216	51.988	-23.704	79.729	1.00	23.78
ATOM	4724	CD2	TYR	B	216	51.970	-21.242	78.439	1.00	19.62
ATOM	4725	CE2	TYR	B	216	52.269	-22.402	77.722	1.00	26.39
ATOM	4726	CZ	TYR	B	216	52.277	-23.630	78.379	1.00	29.35
ATOM	4727	OH	TYR	B	216	52.577	-24.782	77.690	1.00	27.75
ATOM	4728	C	TYR	B	216	52.575	-18.153	81.884	1.00	24.53
ATOM	4729	O	TYR	B	216	52.065	-17.298	81.159	1.00	18.99
ATOM	4730	N	ASN	B	217	53.052	-17.886	83.098	1.00	21.41
ATOM	4731	CA	ASN	B	217	53.073	-16.534	83.642	1.00	21.23
ATOM	4732	CB	ASN	B	217	51.954	-16.325	84.669	1.00	16.78
ATOM	4733	CG	ASN	B	217	51.882	-14.889	85.162	1.00	22.07
ATOM	4734	OD1	ASN	B	217	52.506	-14.521	86.163	1.00	23.13
ATOM	4735	ND2	ASN	B	217	51.146	-14.058	84.435	1.00	19.26
ATOM	4736	C	ASN	B	217	54.437	-16.339	84.291	1.00	19.40
ATOM	4737	O	ASN	B	217	54.857	-17.145	85.124	1.00	19.28
ATOM	4738	N	LEU	B	218	55.130	-15.273	83.905	1.00	18.65
ATOM	4739	CA	LEU	B	218	56.459	-15.004	84.444	1.00	16.41
ATOM	4740	CB	LEU	B	218	57.512	-15.244	83.368	1.00	18.29
ATOM	4741	CG	LEU	B	218	58.851	-15.872	83.782	1.00	28.15
ATOM	4742	CD1	LEU	B	218	59.873	-15.563	82.695	1.00	20.50
ATOM	4743	CD2	LEU	B	218	59.332	-15.348	85.116	1.00	22.53
ATOM	4744	C	LEU	B	218	56.595	-13.562	84.926	1.00	17.89
ATOM	4745	O	LEU	B	218	56.469	-12.627	84.128	1.00	14.48
ATOM	4746	N	ASN	B	219	56.859	-13.395	86.219	1.00	14.09
ATOM	4747	CA	ASN	B	219	57.044	-12.075	86.821	1.00	18.41
ATOM	4748	CB	ASN	B	219	56.238	-11.922	88.111	1.00	14.64
ATOM	4749	CG	ASN	B	219	54.748	-11.898	87.868	1.00	27.12
ATOM	4750	OD1	ASN	B	219	54.286	-11.332	86.880	1.00	20.21
ATOM	4751	ND2	ASN	B	219	53.982	-12.480	88.787	1.00	23.62
ATOM	4752	C	ASN	B	219	58.504	-11.843	87.172	1.00	20.39
ATOM	4753	O	ASN	B	219	59.115	-12.672	87.841	1.00	20.41
ATOM	4754	N	ILE	B	220	59.056	-10.717	86.729	1.00	15.11
ATOM	4755	CA	ILE	B	220	60.441	-10.394	87.033	1.00	17.16
ATOM	4756	CB	ILE	B	220	61.250	-10.083	85.740	1.00	20.78
ATOM	4757	CG2	ILE	B	220	62.736	-9.821	86.094	1.00	18.08
ATOM	4758	CG1	ILE	B	220	61.138	-11.250	84.748	1.00	17.62
ATOM	4759	CD1	ILE	B	220	61.646	-12.590	85.273	1.00	20.72
ATOM	4760	C	ILE	B	220	60.475	-9.161	87.947	1.00	21.17
ATOM	4761	O	ILE	B	220	60.565	-8.036	87.470	1.00	16.03
ATOM	4762	N	PRO	B	221	60.367	-9.357	89.274	1.00	21.74
ATOM	4763	CD	PRO	B	221	60.135	-10.619	90.000	1.00	22.96
ATOM	4764	CA	PRO	B	221	60.394	-8.225	90.213	1.00	19.16
ATOM	4765	CB	PRO	B	221	59.947	-8.869	91.523	1.00	19.40
ATOM	4766	CG	PRO	B	221	60.564	-10.251	91.407	1.00	23.02
ATOM	4767	C	PRO	B	221	61.799	-7.634	90.289	1.00	22.42
ATOM	4768	O	PRO	B	221	62.780	-8.369	90.425	1.00	20.71
ATOM	4769	N	LEU	B	222	61.899	-6.309	90.202	1.00	22.74
ATOM	4770	CA	LEU	B	222	63.198	-5.643	90.223	1.00	21.18
ATOM	4771	CB	LEU	B	222	63.453	-4.993	88.850	1.00	17.21
ATOM	4772	CG	LEU	B	222	63.467	-6.027	87.721	1.00	20.26
ATOM	4773	CD1	LEU	B	222	63.453	-5.354	86.361	1.00	20.00
ATOM	4774	CD2	LEU	B	222	64.696	-6.908	87.881	1.00	21.93
ATOM	4775	C	LEU	B	222	63.335	-4.616	91.353	1.00	20.04

ATOM	4776	O	LEU B 222	62.350	-4.030	91.806	1.00	17.58
ATOM	4777	N	PRO B 223	64.571	-4.394	91.830	1.00	19.48
ATOM	4778	CD	PRO B 223	65.806	-5.072	91.400	1.00	16.80
ATOM	4779	CA	PRO B 223	64.873	-3.454	92.915	1.00	20.38
ATOM	4780	CB	PRO B 223	66.274	-3.881	93.327	1.00	26.11
ATOM	4781	CG	PRO B 223	66.884	-4.161	91.973	1.00	19.74
ATOM	4782	C	PRO B 223	64.818	-1.971	92.553	1.00	21.39
ATOM	4783	C	PRO B 223	64.815	-1.598	91.380	1.00	17.16
ATOM	4784	N	LYS B 224	64.798	-1.142	93.589	1.00	20.65
ATOM	4785	CA	LYS B 224	64.755	0.311	93.462	1.00	27.00
ATOM	4786	CB	LYS B 224	64.577	0.938	94.844	1.00	36.47
ATOM	4787	CG	LYS B 224	63.415	0.389	95.651	1.00	37.72
ATOM	4788	CD	LYS B 224	63.541	0.833	97.101	1.00	42.06
ATOM	4789	CE	LYS B 224	62.420	0.276	97.955	1.00	45.18
ATOM	4790	NZ	LYS B 224	62.645	0.570	99.399	1.00	46.30
ATOM	4791	C	LYS B 224	66.071	0.808	92.874	1.00	27.01
ATOM	4792	O	LYS B 224	67.098	0.139	92.995	1.00	21.54
ATOM	4793	N	GLY B 225	66.038	1.989	92.259	1.00	22.66
ATOM	4794	CA	GLY B 225	67.239	2.565	91.669	1.00	25.67
ATOM	4795	C	GLY B 225	67.768	1.809	90.459	1.00	24.95
ATOM	4796	O	GLY B 225	68.917	1.975	90.069	1.00	26.83
ATOM	4797	N	LEU B 226	66.926	0.980	89.855	1.00	21.79
ATOM	4798	CA	LEU B 226	67.319	0.180	88.692	1.00	22.31
ATOM	4799	CB	LEU B 226	66.067	-0.473	88.099	1.00	23.29
ATOM	4800	CG	LEU B 226	66.238	-1.605	87.091	1.00	26.71
ATOM	4801	CD1	LEU B 226	66.846	-2.804	87.813	1.00	26.44
ATOM	4802	CD2	LEU B 226	64.877	-1.997	86.508	1.00	22.96
ATOM	4803	C	LEU B 226	68.008	1.017	87.603	1.00	22.66
ATOM	4804	O	LEU B 226	67.517	2.087	87.250	1.00	20.19
ATOM	4805	N	ASN B 227	69.134	0.549	87.060	1.00	15.52
ATOM	4806	CA	ASN B 227	69.794	1.317	85.998	1.00	19.49
ATOM	4807	CB	ASN B 227	71.304	1.474	86.270	1.00	20.43
ATOM	4808	CG	ASN B 227	72.062	0.161	86.206	1.00	28.97
ATOM	4809	OD1	ASN B 227	72.015	-0.546	85.199	1.00	24.30
ATOM	4810	ND2	ASN B 227	72.786	-0.160	87.276	1.00	20.88
ATOM	4811	C	ASN B 227	69.548	0.671	84.630	1.00	21.26
ATOM	4812	O	ASN B 227	69.004	-0.432	84.555	1.00	18.90
ATOM	4813	N	ASP B 228	69.949	1.347	83.552	1.00	20.98
ATOM	4814	CA	ASP B 228	69.720	0.817	82.208	1.00	22.61
ATOM	4815	CB	ASP B 228	70.270	1.753	81.126	1.00	23.46
ATOM	4816	CG	ASP B 228	69.596	3.113	81.119	1.00	26.12
ATOM	4817	OD1	ASP B 228	68.387	3.193	81.415	1.00	26.75
ATOM	4818	OD2	ASP B 228	70.276	4.101	80.773	1.00	30.22
ATOM	4819	C	ASP B 228	70.286	-0.573	81.952	1.00	23.49
ATOM	4820	O	ASP B 228	69.651	-1.390	81.288	1.00	19.31
ATOM	4821	N	ASN B 229	71.484	-0.836	82.453	1.00	22.24
ATOM	4822	CA	ASN B 229	72.111	-2.135	82.250	1.00	23.30
ATOM	4823	CB	ASN B 229	73.562	-2.101	82.737	1.00	20.99
ATOM	4824	CG	ASN B 229	74.441	-1.237	81.859	1.00	25.71
ATOM	4825	OD1	ASN B 229	74.644	-1.538	80.678	1.00	26.40
ATOM	4826	ND2	ASN B 229	74.955	-0.151	82.417	1.00	27.44
ATOM	4827	C	ASN B 229	71.341	-3.252	82.943	1.00	23.74
ATOM	4828	O	ASN B 229	71.207	-4.346	82.402	1.00	20.51
ATOM	4829	N	GLU B 230	70.832	-2.976	84.139	1.00	23.06
ATOM	4830	CA	GLU B 230	70.069	-3.977	84.874	1.00	23.01
ATOM	4831	CB	GLU B 230	69.799	-3.480	86.297	1.00	24.73
ATOM	4832	CG	GLU B 230	71.069	-3.201	87.087	1.00	27.28
ATOM	4833	CD	GLU B 230	70.792	-2.649	88.470	1.00	27.47
ATOM	4834	OE1	GLU B 230	70.086	-1.625	88.569	1.00	27.87
ATOM	4835	OE2	GLU B 230	71.286	-3.232	89.455	1.00	26.79
ATOM	4836	C	GLU B 230	68.749	-4.281	84.146	1.00	24.25
ATOM	4837	O	GLU B 230	68.347	-5.445	84.022	1.00	15.89
ATOM	4838	N	PHE B 231	68.091	-3.242	83.637	1.00	21.46
ATOM	4839	CA	PHE B 231	66.814	-3.429	82.933	1.00	22.84
ATOM	4840	CB	PHE B 231	66.210	-2.079	82.529	1.00	23.96
ATOM	4841	CG	PHE B 231	64.803	-2.182	81.975	1.00	26.13

ATOM	4842	CD1	PHE	B	231	63.738	-2.514	82.805	1.00	25.00
ATOM	4843	CD2	PHE	B	231	64.550	-1.956	80.627	1.00	22.93
ATOM	4844	CE1	PHE	B	231	62.440	-2.618	82.304	1.00	25.03
ATOM	4845	CE2	PHE	B	231	63.250	-2.059	80.114	1.00	27.46
ATOM	4846	CZ	PHE	B	231	62.196	-2.390	80.957	1.00	20.25
ATOM	4847	C	PHE	B	231	66.978	-4.288	81.677	1.00	23.14
ATOM	4848	O	PHE	B	231	66.221	-5.239	81.464	1.00	20.02
ATOM	4849	N	LEU	B	232	67.963	-3.952	80.845	1.00	22.02
ATOM	4850	CA	LEU	B	232	68.200	-4.697	79.614	1.00	19.97
ATOM	4851	CB	LEU	B	232	69.192	-3.942	78.734	1.00	24.99
ATOM	4852	CG	LEU	B	232	68.665	-2.581	78.263	1.00	29.73
ATOM	4853	CD1	LEU	B	232	69.746	-1.856	77.454	1.00	28.11
ATOM	4854	CD2	LEU	B	232	67.409	-2.784	77.414	1.00	26.54
ATOM	4855	C	LEU	B	232	68.688	-6.119	79.898	1.00	19.25
ATOM	4856	O	LEU	B	232	68.365	-7.051	79.162	1.00	19.49
ATOM	4857	N	PHE	B	233	69.468	-6.280	80.962	1.00	20.50
ATOM	4858	CA	PHE	B	233	69.950	-7.599	81.378	1.00	20.70
ATOM	4859	CB	PHE	B	233	70.825	-7.471	82.632	1.00	23.75
ATOM	4860	CG	PHE	B	233	71.217	-8.790	83.239	1.00	28.58
ATOM	4861	CD1	PHE	B	233	72.285	-9.519	82.731	1.00	30.48
ATOM	4862	CD2	PHE	B	233	70.481	-9.328	84.294	1.00	25.32
ATOM	4863	CE1	PHE	B	233	72.617	-10.762	83.262	1.00	31.87
ATOM	4864	CE2	PHE	B	233	70.803	-10.573	84.832	1.00	31.26
ATOM	4865	CZ	PHE	B	233	71.871	-11.292	84.317	1.00	32.29
ATOM	4866	C	PHE	B	233	68.712	-8.439	81.727	1.00	20.23
ATOM	4867	O	PHE	B	233	68.553	-9.567	81.270	1.00	21.56
ATOM	4868	N	ALA	B	234	67.842	-7.878	82.560	1.00	21.26
ATOM	4869	CA	ALA	B	234	66.626	-8.576	82.963	1.00	19.60
ATOM	4870	CB	ALA	B	234	65.835	-7.733	83.950	1.00	19.25
ATOM	4871	C	ALA	B	234	65.772	-8.898	81.749	1.00	18.87
ATOM	4872	O	ALA	B	234	65.253	-10.010	81.624	1.00	21.91
ATOM	4873	N	LEU	B	235	65.634	-7.934	80.845	1.00	20.29
ATOM	4874	CA	LEU	B	235	64.822	-8.141	79.652	1.00	19.53
ATOM	4875	CB	LEU	B	235	64.773	-6.874	78.795	1.00	24.07
ATOM	4876	CG	LEU	B	235	63.465	-6.607	78.024	1.00	27.87
ATOM	4877	CD1	LEU	B	235	63.783	-5.813	76.770	1.00	20.77
ATOM	4878	CD2	LEU	B	235	62.761	-7.897	77.664	1.00	26.94
ATOM	4879	C	LEU	B	235	65.376	-9.276	78.795	1.00	20.79
ATOM	4880	O	LEU	B	235	64.648	-10.205	78.431	1.00	18.25
ATOM	4881	N	GLU	B	236	66.665	-9.191	78.462	1.00	19.33
ATOM	4882	CA	GLU	B	236	67.303	-10.206	77.629	1.00	27.93
ATOM	4883	CB	GLU	B	236	68.777	-9.853	77.384	1.00	31.06
ATOM	4884	CG	GLU	B	236	68.969	-8.597	76.548	1.00	43.60
ATOM	4885	CD	GLU	B	236	70.428	-8.292	76.259	1.00	45.19
ATOM	4886	OE1	GLU	B	236	70.697	-7.309	75.538	1.00	48.77
ATOM	4887	OE2	GLU	B	236	71.307	-9.032	76.751	1.00	52.72
ATOM	4888	C	GLU	B	236	67.201	-11.607	78.209	1.00	24.89
ATOM	4889	O	GLU	B	236	66.861	-12.552	77.501	1.00	22.06
ATOM	4890	N	LYS	B	237	67.520	-11.748	79.492	1.00	24.20
ATOM	4891	CA	LYS	B	237	67.449	-13.058	80.130	1.00	27.10
ATOM	4892	CB	LYS	B	237	67.989	-12.984	81.562	1.00	23.43
ATOM	4893	CG	LYS	B	237	69.466	-12.641	81.650	1.00	29.46
ATOM	4894	CD	LYS	B	237	70.305	-13.683	80.924	1.00	31.65
ATOM	4895	CE	LYS	B	237	71.782	-13.356	80.993	1.00	39.70
ATOM	4896	NZ	LYS	B	237	72.580	-14.363	80.242	1.00	46.74
ATOM	4897	C	LYS	B	237	66.019	-13.615	80.143	1.00	30.92
ATOM	4898	O	LYS	B	237	65.789	-14.766	79.763	1.00	31.42
ATOM	4899	N	SER	B	238	65.057	-12.806	80.573	1.00	25.86
ATOM	4900	CA	SER	B	238	63.677	-13.280	80.620	1.00	27.98
ATOM	4901	CB	SER	B	238	62.776	-12.241	81.289	1.00	23.89
ATOM	4902	OG	SER	B	238	62.756	-11.028	80.565	1.00	29.27
ATOM	4903	C	SER	B	238	63.145	-13.642	79.229	1.00	28.32
ATOM	4904	O	SER	B	238	62.387	-14.605	79.089	1.00	29.65
ATOM	4905	N	LEU	B	239	63.536	-12.886	78.203	1.00	27.39
ATOM	4906	CA	LEU	B	239	63.079	-13.192	76.846	1.00	32.52
ATOM	4907	CB	LEU	B	239	63.544	-12.129	75.837	1.00	30.53

ATOM	4908	CG	LEU	B	239	62.833	-10.772	75.895	1.00	36.06
ATOM	4909	CD1	LEU	B	239	63.404	-9.836	74.842	1.00	29.64
ATOM	4910	CD2	LEU	B	239	61.338	-10.976	75.667	1.00	30.73
ATOM	4911	C	LEU	B	239	63.598	-14.563	76.430	1.00	34.15
ATOM	4912	O	LEU	B	239	62.879	-15.340	75.803	1.00	33.23
ATOM	4913	N	GLU	B	240	64.844	-14.859	76.788	1.00	31.39
ATOM	4914	CA	GLU	B	240	65.434	-16.152	76.472	1.00	33.79
ATOM	4915	CB	GLU	B	240	66.859	-16.238	77.011	1.00	38.51
ATOM	4916	CG	GLU	B	240	67.878	-15.407	76.275	1.00	40.56
ATOM	4917	CD	GLU	B	240	69.256	-15.532	76.903	1.00	48.20
ATOM	4918	OE1	GLU	B	240	69.685	-16.679	77.161	1.00	45.36
ATOM	4919	OE2	GLU	B	240	69.912	-14.492	77.130	1.00	48.21
ATOM	4920	C	GLU	B	240	64.604	-17.258	77.108	1.00	33.23
ATOM	4921	O	GLU	B	240	64.391	-18.310	76.510	1.00	32.15
ATOM	4922	N	ILE	B	241	64.146	-17.017	78.331	1.00	29.72
ATOM	4923	CA	ILE	B	241	63.328	-17.989	79.047	1.00	29.85
ATOM	4924	CB	ILE	B	241	63.006	-17.489	80.466	1.00	30.42
ATOM	4925	CG2	ILE	B	241	62.049	-18.456	81.162	1.00	29.88
ATOM	4926	CG1	ILE	B	241	64.309	-17.311	81.254	1.00	29.77
ATOM	4927	CD1	ILE	B	241	64.118	-16.760	82.654	1.00	32.92
ATOM	4928	C	ILE	B	241	62.016	-18.247	78.298	1.00	34.65
ATOM	4929	O	ILE	B	241	61.592	-19.396	78.149	1.00	30.22
ATOM	4930	N	VAL	B	242	61.379	-17.178	77.823	1.00	31.16
ATOM	4931	CA	VAL	B	242	60.114	-17.312	77.105	1.00	34.55
ATOM	4932	CB	VAL	B	242	59.476	-15.937	76.825	1.00	30.77
ATOM	4933	CG1	VAL	B	242	58.191	-16.113	76.038	1.00	32.18
ATOM	4934	CG2	VAL	B	242	59.201	-15.214	78.140	1.00	31.57
ATOM	4935	C	VAL	B	242	60.320	-18.042	75.787	1.00	36.56
ATOM	4936	O	VAL	B	242	59.572	-18.959	75.453	1.00	33.93
ATOM	4937	N	LYS	B	243	61.337	-17.627	75.042	1.00	38.64
ATOM	4938	CA	LYS	B	243	61.659	-18.241	73.760	1.00	44.36
ATOM	4939	CB	LYS	B	243	62.966	-17.659	73.214	1.00	48.33
ATOM	4940	CG	LYS	B	243	62.810	-16.399	72.386	1.00	53.88
ATOM	4941	CD	LYS	B	243	62.185	-16.718	71.036	1.00	53.72
ATOM	4942	CE	LYS	B	243	63.056	-17.681	70.242	1.00	54.69
ATOM	4943	NZ	LYS	B	243	62.456	-18.025	68.923	1.00	57.75
ATOM	4944	C	LYS	B	243	61.793	-19.755	73.824	1.00	43.21
ATOM	4945	O	LYS	B	243	61.432	-20.455	72.884	1.00	42.92
ATOM	4946	N	GLU	B	244	62.312	-20.257	74.935	1.00	45.77
ATOM	4947	CA	GLU	B	244	62.528	-21.687	75.085	1.00	47.72
ATOM	4948	CB	GLU	B	244	63.669	-21.925	76.075	1.00	50.89
ATOM	4949	CG	GLU	B	244	64.080	-23.378	76.208	1.00	57.16
ATOM	4950	CD	GLU	B	244	65.223	-23.564	77.173	1.00	57.74
ATOM	4951	OE1	GLU	B	244	66.295	-22.967	76.942	1.00	60.18
ATOM	4952	OE2	GLU	B	244	65.049	-24.308	78.160	1.00	61.59
ATOM	4953	C	GLU	B	244	61.312	-22.507	75.505	1.00	47.78
ATOM	4954	O	GLU	B	244	61.376	-23.736	75.544	1.00	51.39
ATOM	4955	N	VAL	B	245	60.200	-21.851	75.805	1.00	43.31
ATOM	4956	CA	VAL	B	245	59.019	-22.589	76.230	1.00	43.55
ATOM	4957	CB	VAL	B	245	58.867	-22.514	77.771	1.00	45.89
ATOM	4958	CG1	VAL	B	245	57.665	-23.322	78.231	1.00	49.90
ATOM	4959	CG2	VAL	B	245	60.131	-23.040	78.435	1.00	46.37
ATOM	4960	C	VAL	B	245	57.727	-22.115	75.565	1.00	41.01
ATOM	4961	O	VAL	B	245	56.659	-22.676	75.798	1.00	39.36
ATOM	4962	N	PHE	B	246	57.814	-21.101	74.716	1.00	34.37
ATOM	4963	CA	PHE	B	246	56.610	-20.602	74.077	1.00	34.36
ATOM	4964	CB	PHE	B	246	55.986	-19.517	74.958	1.00	30.80
ATOM	4965	CG	PHE	B	246	54.542	-19.230	74.644	1.00	32.57
ATOM	4966	CD1	PHE	B	246	53.548	-20.142	74.989	1.00	27.72
ATOM	4967	CD2	PHE	B	246	54.174	-18.048	74.003	1.00	28.20
ATOM	4968	CE1	PHE	B	246	52.207	-19.878	74.704	1.00	26.71
ATOM	4969	CE2	PHE	B	246	52.836	-17.773	73.713	1.00	29.27
ATOM	4970	CD	PHE	B	246	51.850	-18.689	74.065	1.00	26.18
ATOM	4971	C	PHE	B	246	56.904	-20.040	72.682	1.00	35.32
ATOM	4972	O	PHE	B	246	57.740	-19.153	72.517	1.00	31.73
ATOM	4973	N	GLU	B	247	56.205	-20.568	71.683	1.00	37.00

ATOM	4974	CA	GLU	B	247	56.363	-20.137	70.296	1.00	40.73
ATOM	4975	CB	GLU	B	247	56.518	-21.347	69.370	1.00	43.38
ATOM	4976	CG	GLU	B	247	56.670	-22.702	70.073	1.00	51.49
ATOM	4977	CD	GLU	B	247	55.381	-23.214	70.718	1.00	55.29
ATOM	4978	OE1	GLU	B	247	54.887	-22.601	71.691	1.00	49.08
ATOM	4979	OE2	GLU	B	247	54.859	-24.246	70.241	1.00	60.95
ATOM	4980	C	GLU	B	247	55.090	-19.379	69.939	1.00	39.04
ATOM	4981	O	GLU	B	247	54.129	-19.960	69.436	1.00	39.49
ATOM	4982	N	PRO	B	248	55.076	-18.064	70.182	1.00	35.13
ATOM	4983	CD	PRO	B	248	56.188	-17.270	70.733	1.00	33.57
ATOM	4984	CA	PRO	B	248	53.935	-17.188	69.916	1.00	36.03
ATOM	4985	CB	PRO	B	248	54.375	-15.878	70.562	1.00	35.33
ATOM	4986	CG	PRO	B	248	55.844	-15.880	70.233	1.00	32.85
ATOM	4987	C	PRO	B	248	53.563	-16.990	68.457	1.00	33.44
ATOM	4988	O	PRO	B	248	54.427	-16.808	67.604	1.00	29.38
ATOM	4989	N	GLU	B	249	52.263	-17.012	68.182	1.00	32.23
ATOM	4990	CA	GLU	B	249	51.773	-16.782	66.828	1.00	29.35
ATOM	4991	CB	GLU	B	249	50.374	-17.366	66.645	1.00	31.87
ATOM	4992	CG	GLU	B	249	50.284	-18.867	66.787	1.00	28.64
ATOM	4993	CD	GLU	B	249	48.847	-19.338	66.747	1.00	33.37
ATOM	4994	OE1	GLU	B	249	48.069	-18.917	67.630	1.00	26.38
ATOM	4995	OE2	GLU	B	249	48.494	-20.115	65.835	1.00	37.71
ATOM	4996	C	GLU	B	249	51.700	-15.273	66.650	1.00	28.25
ATOM	4997	O	GLU	B	249	51.776	-14.765	65.537	1.00	21.47
ATOM	4998	N	VAL	B	250	51.561	-14.564	67.768	1.00	21.77
ATOM	4999	CA	VAL	B	250	51.459	-13.110	67.756	1.00	21.41
ATOM	5000	CB	VAL	B	250	50.027	-12.676	67.357	1.00	26.42
ATOM	5001	CG1	VAL	B	250	49.037	-13.196	68.378	1.00	20.96
ATOM	5002	CG2	VAL	B	250	49.931	-11.166	67.243	1.00	24.68
ATOM	5003	C	VAL	B	250	51.757	-12.608	69.168	1.00	22.88
ATOM	5004	O	VAL	B	250	51.592	-13.354	70.133	1.00	18.00
ATOM	5005	N	TYR	B	251	52.201	-11.359	69.295	1.00	20.28
ATOM	5006	CA	TYR	B	251	52.481	-10.823	70.620	1.00	22.33
ATOM	5007	CB	TYR	B	251	53.956	-11.043	70.999	1.00	20.67
ATOM	5008	CG	TYR	B	251	54.948	-10.045	70.427	1.00	21.89
ATOM	5009	CD1	TYR	B	251	55.198	-8.834	71.072	1.00	19.31
ATOM	5010	CE1	TYR	B	251	56.129	-7.922	70.562	1.00	23.73
ATOM	5011	CD2	TYR	B	251	55.651	-10.321	69.254	1.00	18.72
ATOM	5012	CE2	TYR	B	251	56.580	-9.417	68.734	1.00	22.71
ATOM	5013	CZ	TYR	B	251	56.813	-8.220	69.390	1.00	27.33
ATOM	5014	OH	TYR	B	251	57.705	-7.308	68.865	1.00	23.18
ATOM	5015	C	TYR	B	251	52.134	-9.349	70.732	1.00	25.71
ATOM	5016	O	TYR	B	251	52.095	-8.622	69.728	1.00	20.14
ATOM	5017	N	LEU	B	252	51.834	-8.930	71.958	1.00	21.13
ATOM	5018	CA	LEU	B	252	51.533	-7.532	72.252	1.00	24.61
ATOM	5019	CB	LEU	B	252	50.154	-7.373	72.897	1.00	22.88
ATOM	5020	CG	LEU	B	252	48.915	-7.435	71.996	1.00	23.73
ATOM	5021	CD1	LEU	B	252	48.779	-8.792	71.360	1.00	23.18
ATOM	5022	CD2	LEU	B	252	47.697	-7.119	72.833	1.00	29.06
ATOM	5023	C	LEU	B	252	52.610	-7.044	73.217	1.00	24.77
ATOM	5024	O	LEU	B	252	53.064	-7.797	74.076	1.00	23.33
ATOM	5025	N	LEU	B	253	53.011	-5.786	73.071	1.00	20.14
ATOM	5026	CA	LEU	B	253	54.057	-5.209	73.911	1.00	20.33
ATOM	5027	CB	LEU	B	253	55.304	-4.946	73.051	1.00	15.18
ATOM	5028	CG	LEU	B	253	56.490	-4.210	73.688	1.00	18.34
ATOM	5029	CD1	LEU	B	253	57.062	-5.044	74.829	1.00	14.11
ATOM	5030	CD2	LEU	B	253	57.552	-3.953	72.624	1.00	19.60
ATOM	5031	C	LEU	B	253	53.550	-3.913	74.536	1.00	20.54
ATOM	5032	O	LEU	B	253	53.200	-2.974	73.821	1.00	22.80
ATOM	5033	N	GLN	B	254	53.495	-3.858	75.865	1.00	20.37
ATOM	5034	CA	GLN	B	254	53.000	-2.654	76.539	1.00	21.77
ATOM	5035	CB	GLN	B	254	52.129	-3.040	77.755	1.00	17.85
ATOM	5036	CG	GLN	B	254	52.724	-2.815	79.124	1.00	32.51
ATOM	5037	CD	GLN	B	254	52.563	-1.396	79.609	1.00	28.19
ATOM	5038	OE1	GLN	B	254	51.507	-0.996	80.124	1.00	26.96
ATOM	5039	NE2	GLN	B	254	53.603	-0.619	79.432	1.00	16.80

Figure 18-77

ATOM	5040	C	GLN	B	254	54.211	-1.793	76.887	1.00	20.15
ATOM	5041	O	GLN	B	254	55.186	-2.254	77.497	1.00	20.11
ATOM	5042	N	LEU	B	255	54.146	-0.532	76.468	1.00	19.46
ATOM	5043	CA	LEU	B	255	55.268	0.386	76.614	1.00	15.99
ATOM	5044	CB	LEU	B	255	55.692	0.831	75.211	1.00	18.15
ATOM	5045	CG	LEU	B	255	56.143	-0.316	74.296	1.00	21.80
ATOM	5046	CD1	LEU	B	255	56.215	0.159	72.850	1.00	16.70
ATOM	5047	CD2	LEU	B	255	57.501	-0.843	74.771	1.00	13.76
ATOM	5048	C	LEU	B	255	55.083	1.614	77.492	1.00	21.41
ATOM	5049	O	LEU	B	255	55.379	2.741	77.065	1.00	18.40
ATOM	5050	N	GLY	B	256	54.618	1.408	78.718	1.00	16.80
ATOM	5051	CA	GLY	B	256	54.456	2.519	79.634	1.00	19.90
ATOM	5052	C	GLY	B	256	55.816	3.181	79.818	1.00	17.68
ATOM	5053	O	GLY	B	256	56.854	2.514	79.841	1.00	13.96
ATOM	5054	N	THR	B	257	55.824	4.497	79.936	1.00	19.55
ATOM	5055	CA	THR	B	257	57.081	5.205	80.098	1.00	19.47
ATOM	5056	CB	THR	B	257	57.044	6.547	79.340	1.00	21.49
ATOM	5057	OG1	THR	B	257	55.989	7.365	79.858	1.00	17.43
ATOM	5058	CG2	THR	B	257	56.780	6.311	77.850	1.00	22.49
ATOM	5059	C	THR	B	257	57.440	5.466	81.564	1.00	20.75
ATOM	5060	O	THR	B	257	58.480	5.054	81.843	1.00	25.01
ATOM	5061	N	ASP	B	258	56.618	5.004	82.504	1.00	17.23
ATOM	5062	CA	ASP	B	258	56.929	5.277	83.906	1.00	17.42
ATOM	5063	CB	ASP	B	258	55.744	4.940	84.846	1.00	12.75
ATOM	5064	CG	ASP	B	258	55.197	3.524	84.676	1.00	21.60
ATOM	5065	C	ASP	B	258	58.245	4.718	84.460	1.00	16.09
ATOM	5066	O	ASP	B	258	58.667	5.116	85.542	1.00	22.07
ATOM	5067	OD1	ASP	B	258	55.901	2.642	84.150	1.00	17.74
ATOM	5068	OD2	ASP	B	258	54.041	3.281	85.109	1.00	18.68
ATOM	5069	N	PRO	B	259	58.879	3.746	83.779	1.00	20.98
ATOM	5070	CD	PRO	B	259	58.474	2.901	82.641	1.00	17.75
ATOM	5071	CA	PRO	B	259	60.154	3.257	84.321	1.00	22.63
ATOM	5072	CB	PRO	B	259	60.395	1.988	83.506	1.00	23.46
ATOM	5073	CG	PRO	B	259	59.800	2.343	82.199	1.00	27.08
ATOM	5074	C	PRO	B	259	61.305	4.284	84.172	1.00	23.86
ATOM	5075	O	PRO	B	259	62.406	4.082	84.698	1.00	24.24
ATOM	5076	N	LEU	B	260	61.054	5.387	83.465	1.00	20.49
ATOM	5077	CA	LEU	B	260	62.080	6.417	83.262	1.00	15.17
ATOM	5078	CB	LEU	B	260	61.626	7.408	82.185	1.00	17.03
ATOM	5079	CG	LEU	B	260	61.431	6.881	80.760	1.00	16.02
ATOM	5080	CD1	LEU	B	260	60.703	7.915	79.901	1.00	17.03
ATOM	5081	CD2	LEU	B	260	62.803	6.546	80.163	1.00	18.58
ATOM	5082	C	LEU	B	260	62.449	7.194	84.541	1.00	22.45
ATOM	5083	O	LEU	B	260	61.611	7.440	85.412	1.00	17.84
ATOM	5084	N	LEU	B	261	63.713	7.588	84.635	1.00	22.90
ATOM	5085	CA	LEU	B	261	64.219	8.332	85.782	1.00	26.34
ATOM	5086	CB	LEU	B	261	65.605	8.914	85.473	1.00	20.58
ATOM	5087	CG	LEU	B	261	66.180	9.850	86.553	1.00	28.44
ATOM	5088	CD1	LEU	B	261	66.481	9.055	87.812	1.00	29.84
ATOM	5089	CD2	LEU	B	261	67.462	10.522	86.057	1.00	32.10
ATOM	5090	C	LEU	B	261	63.315	9.475	86.227	1.00	27.61
ATOM	5091	O	LEU	B	261	62.978	9.586	87.408	1.00	24.02
ATOM	5092	N	GLU	B	262	62.934	10.315	85.269	1.00	23.33
ATOM	5093	CA	GLU	B	262	62.126	11.490	85.530	1.00	23.38
ATOM	5094	CB	GLU	B	262	62.115	12.415	84.302	1.00	23.17
ATOM	5095	CG	GLU	B	262	63.503	12.854	83.806	1.00	28.98
ATOM	5096	CD	GLU	B	262	64.179	11.831	82.902	1.00	32.26
ATOM	5097	OE1	GLU	B	262	63.702	10.673	82.838	1.00	29.28
ATOM	5098	OE2	GLU	B	262	65.201	12.186	82.264	1.00	25.42
ATOM	5099	C	GLU	B	262	60.693	11.249	85.976	1.00	23.25
ATOM	5100	O	GLU	B	262	60.013	12.192	86.368	1.00	27.63
ATOM	5101	N	ASP	B	263	60.219	10.011	85.927	1.00	22.25
ATOM	5102	CA	ASP	B	263	58.840	9.751	86.345	1.00	24.46
ATOM	5103	CB	ASP	B	263	58.214	8.659	85.465	1.00	20.94
ATOM	5104	CG	ASP	B	263	56.710	8.543	85.659	1.00	25.30
ATOM	5105	OD1	ASP	B	263	55.995	8.318	84.656	1.00	21.82

Figure 18-78

ATOM	5106	OD2	ASP	B	263	56.239	8.666	86.811	1.00	18.31
ATOM	5107	C	ASP	B	263	58.834	9.339	87.814	1.00	26.39
ATOM	5108	O	ASP	B	263	59.437	8.335	88.179	1.00	22.11
ATOM	5109	N	TYR	B	264	58.155	10.124	88.648	1.00	25.81
ATOM	5110	CA	TYR	B	264	58.101	9.864	90.084	1.00	30.96
ATOM	5111	CB	TYR	B	264	57.511	11.055	90.841	1.00	36.80
ATOM	5112	CG	TYR	B	264	58.241	12.356	90.645	1.00	46.58
ATOM	5113	CD1	TYR	B	264	57.981	13.166	89.542	1.00	47.03
ATOM	5114	CE1	TYR	B	264	58.654	14.370	89.364	1.00	50.25
ATOM	5115	CD2	TYR	B	264	59.197	12.779	91.565	1.00	50.94
ATOM	5116	CE2	TYR	B	264	59.876	13.977	91.396	1.00	51.28
ATOM	5117	CZ	TYR	B	264	59.600	14.769	90.297	1.00	52.21
ATOM	5118	OH	TYR	B	264	60.268	15.961	90.142	1.00	49.65
ATOM	5119	C	TYR	B	264	57.340	8.628	90.525	1.00	31.04
ATOM	5120	O	TYR	B	264	57.514	8.181	91.657	1.00	24.50
ATOM	5121	N	LEU	B	265	56.491	8.074	89.666	1.00	26.68
ATOM	5122	CA	LEU	B	265	55.744	6.900	90.086	1.00	24.17
ATOM	5123	CB	LEU	B	265	54.371	6.838	89.390	1.00	24.69
ATOM	5124	CG	LEU	B	265	53.415	7.982	89.761	1.00	26.00
ATOM	5125	CD1	LEU	B	265	51.970	7.583	89.460	1.00	22.21
ATOM	5126	CD2	LEU	B	265	53.530	8.281	91.238	1.00	29.31
ATOM	5127	C	LEU	B	265	56.478	5.568	89.948	1.00	25.83
ATOM	5128	O	LEU	B	265	55.848	4.512	89.908	1.00	21.74
ATOM	5129	N	SER	B	266	57.808	5.618	89.867	1.00	23.30
ATOM	5130	CA	SER	B	266	58.608	4.398	89.813	1.00	20.75
ATOM	5131	CB	SER	B	266	58.820	3.900	88.378	1.00	19.67
ATOM	5132	OG	SER	B	266	59.863	4.615	87.739	1.00	18.11
ATOM	5133	C	SER	B	266	59.963	4.710	90.420	1.00	23.01
ATOM	5134	O	SER	B	266	60.437	5.845	90.345	1.00	17.74
ATOM	5135	N	LYS	B	267	60.590	3.707	91.023	1.00	24.25
ATOM	5136	CA	LYS	B	267	61.905	3.916	91.613	1.00	23.79
ATOM	5137	CB	LYS	B	267	62.027	3.153	92.929	1.00	23.71
ATOM	5138	CG	LYS	B	267	60.989	3.582	93.960	1.00	27.29
ATOM	5139	CD	LYS	B	267	61.059	5.088	94.207	1.00	30.33
ATOM	5140	CE	LYS	B	267	60.067	5.535	95.273	1.00	30.90
ATOM	5141	NZ	LYS	B	267	60.155	7.004	95.509	1.00	33.37
ATOM	5142	C	LYS	B	267	62.990	3.483	90.634	1.00	26.41
ATOM	5143	O	LYS	B	267	64.153	3.317	91.016	1.00	25.33
ATOM	5144	N	PHE	B	268	62.595	3.288	89.375	1.00	22.18
ATOM	5145	CA	PHE	B	268	63.529	2.919	88.318	1.00	22.78
ATOM	5146	CB	PHE	B	268	62.814	2.171	87.179	1.00	20.55
ATOM	5147	CG	PHE	B	268	62.389	0.761	87.526	1.00	19.23
ATOM	5148	CD1	PHE	B	268	61.722	-0.025	86.585	1.00	20.72
ATOM	5149	CD2	PHE	B	268	62.673	0.207	88.773	1.00	18.17
ATOM	5150	CE1	PHE	B	268	61.344	-1.336	86.875	1.00	18.83
ATOM	5151	CE2	PHE	B	268	62.300	-1.105	89.073	1.00	20.05
ATOM	5152	CZ	PHE	B	268	61.634	-1.879	88.122	1.00	19.70
ATOM	5153	C	PHE	B	268	64.114	4.222	87.785	1.00	23.66
ATOM	5154	O	PHE	B	268	63.412	5.232	87.692	1.00	19.40
ATOM	5155	N	ASN	B	269	65.396	4.203	87.437	1.00	21.96
ATOM	5156	CA	ASN	B	269	66.060	5.396	86.926	1.00	25.04
ATOM	5157	CB	ASN	B	269	67.243	5.783	87.824	1.00	25.68
ATOM	5158	CG	ASN	B	269	66.845	5.946	89.273	1.00	27.04
ATOM	5159	OD1	ASN	B	269	65.832	6.557	89.579	1.00	28.81
ATOM	5160	ND2	ASN	B	269	67.659	5.419	90.176	1.00	31.12
ATOM	5161	C	ASN	B	269	66.579	5.151	85.523	1.00	25.87
ATOM	5162	O	ASN	B	269	67.769	5.336	85.268	1.00	24.58
ATOM	5163	N	LEU	B	270	65.695	4.757	84.611	1.00	21.37
ATOM	5164	CA	LEU	B	270	66.116	4.462	83.241	1.00	16.35
ATOM	5165	CB	LEU	B	270	65.176	3.426	82.610	1.00	24.12
ATOM	5166	CG	LEU	B	270	64.909	2.144	83.412	1.00	27.89
ATOM	5167	CD1	LEU	B	270	64.181	1.136	82.515	1.00	23.01
ATOM	5168	CD2	LEU	B	270	66.221	1.547	83.904	1.00	23.92
ATOM	5169	C	LEU	B	270	66.184	5.682	82.337	1.00	20.06
ATOM	5170	O	LEU	B	270	65.654	6.761	82.663	1.00	16.34
ATOM	5171	N	SER	B	271	66.839	5.497	81.193	1.00	20.07

Figure 18-79

ATOM	5172	CA	SER	B	271	66.989	6.546	80.200	1.00	21.20
ATOM	5173	CB	SER	B	271	68.437	6.621	79.714	1.00	21.80
ATOM	5174	OG	SER	B	271	68.772	5.485	78.921	1.00	21.47
ATOM	5175	C	SER	B	271	66.106	6.228	79.000	1.00	22.83
ATOM	5176	O	SER	B	271	65.631	5.102	78.854	1.00	16.12
ATOM	5177	N	ASN	B	272	65.916	7.238	78.154	1.00	20.84
ATOM	5178	CA	ASN	B	272	65.152	7.156	76.906	1.00	27.82
ATOM	5179	CB	ASN	B	272	65.263	8.478	76.123	1.00	30.30
ATOM	5180	CG	ASN	B	272	64.198	9.456	76.475	1.00	37.83
ATOM	5181	OD1	ASN	B	272	64.167	10.575	75.946	1.00	37.72
ATOM	5182	ND2	ASN	B	272	63.299	9.052	77.360	1.00	41.69
ATOM	5183	C	ASN	B	272	65.701	6.088	75.974	1.00	26.88
ATOM	5184	O	ASN	B	272	64.967	5.280	75.412	1.00	23.12
ATOM	5185	N	VAL	B	273	67.012	6.160	75.774	1.00	20.40
ATOM	5186	CA	VAL	B	273	67.745	5.260	74.899	1.00	27.34
ATOM	5187	CB	VAL	B	273	69.225	5.705	74.805	1.00	30.40
ATOM	5188	CG1	VAL	B	273	70.036	4.691	74.029	1.00	34.98
ATOM	5189	CG2	VAL	B	273	69.299	7.057	74.115	1.00	33.57
ATOM	5190	C	VAL	B	273	67.664	3.812	75.343	1.00	24.23
ATOM	5191	O	VAL	B	273	67.590	2.913	74.513	1.00	24.19
ATOM	5192	N	ALA	B	274	67.690	3.580	76.648	1.00	20.96
ATOM	5193	CA	ALA	B	274	67.589	2.220	77.151	1.00	18.12
ATOM	5194	CB	ALA	B	274	67.858	2.195	78.646	1.00	19.09
ATOM	5195	C	ALA	B	274	66.172	1.729	76.863	1.00	18.23
ATOM	5196	O	ALA	B	274	65.962	0.567	76.525	1.00	20.77
ATOM	5197	N	PHE	B	275	65.207	2.631	77.003	1.00	18.50
ATOM	5198	CA	PHE	B	275	63.802	2.310	76.761	1.00	21.25
ATOM	5199	CB	PHE	B	275	62.941	3.546	77.037	1.00	22.24
ATOM	5200	CG	PHE	B	275	61.466	3.303	76.921	1.00	24.72
ATOM	5201	CD1	PHE	B	275	60.815	2.483	77.826	1.00	23.64
ATOM	5202	CD2	PHE	B	275	60.732	3.893	75.907	1.00	27.31
ATOM	5203	CE1	PHE	B	275	59.450	2.254	77.722	1.00	27.82
ATOM	5204	CE2	PHE	B	275	59.365	3.670	75.795	1.00	27.62
ATOM	5205	CZ	PHE	B	275	58.727	2.851	76.701	1.00	25.78
ATOM	5206	C	PHE	B	275	63.642	1.860	75.305	1.00	24.47
ATOM	5207	O	PHE	B	275	63.045	0.821	75.030	1.00	22.68
ATOM	5208	N	LEU	B	276	64.183	2.648	74.378	1.00	23.85
ATOM	5209	CA	LEU	B	276	64.128	2.330	72.946	1.00	21.28
ATOM	5210	CB	LEU	B	276	64.814	3.421	72.134	1.00	19.87
ATOM	5211	CG	LEU	B	276	65.114	3.132	70.662	1.00	24.94
ATOM	5212	CD1	LEU	B	276	63.818	2.852	69.936	1.00	24.81
ATOM	5213	CD2	LEU	B	276	65.840	4.312	70.018	1.00	21.01
ATOM	5214	C	LEU	B	276	64.841	1.021	72.653	1.00	22.33
ATOM	5215	O	LEU	B	276	64.348	0.191	71.886	1.00	20.73
ATOM	5216	N	LYS	B	277	66.011	0.857	73.261	1.00	20.72
ATOM	5217	CA	LYS	B	277	66.823	-0.335	73.076	1.00	24.36
ATOM	5218	CB	LYS	B	277	68.086	-0.239	73.938	1.00	27.37
ATOM	5219	CG	LYS	B	277	69.303	-0.973	73.381	1.00	35.58
ATOM	5220	CD	LYS	B	277	69.061	-2.456	73.188	1.00	43.87
ATOM	5221	CE	LYS	B	277	70.283	-3.137	72.580	1.00	44.87
ATOM	5222	NZ	LYS	B	277	70.616	-2.586	71.230	1.00	49.66
ATOM	5223	C	LYS	B	277	66.000	-1.554	73.482	1.00	24.22
ATOM	5224	O	LYS	B	277	65.987	-2.568	72.777	1.00	19.90
ATOM	5225	N	ALA	B	278	65.319	-1.454	74.624	1.00	22.32
ATOM	5226	CA	ALA	B	278	64.476	-2.544	75.114	1.00	21.71
ATOM	5227	CB	ALA	B	278	63.752	-2.117	76.381	1.00	17.34
ATOM	5228	C	ALA	B	278	63.459	-2.896	74.031	1.00	22.68
ATOM	5229	O	ALA	B	278	63.231	-4.068	73.723	1.00	19.27
ATOM	5230	N	PHE	B	279	62.849	-1.862	73.464	1.00	24.79
ATOM	5231	CA	PHE	B	279	61.860	-2.014	72.398	1.00	22.74
ATOM	5232	CB	PHE	B	279	61.395	-0.629	71.955	1.00	22.46
ATOM	5233	CG	PHE	B	279	60.467	-0.640	70.778	1.00	22.62
ATOM	5234	CD1	PHE	B	279	59.196	-1.182	70.882	1.00	21.74
ATOM	5235	CD2	PHE	B	279	60.862	-0.078	69.567	1.00	26.07
ATOM	5236	CE1	PHE	B	279	58.325	-1.162	69.799	1.00	27.02
ATOM	5237	CE2	PHE	B	279	60.001	-0.051	68.476	1.00	25.57

ATOM	5238	CZ	PHE	B	279	58.727	-0.594	68.592	1.00	25.13
ATOM	5239	C	PHE	B	279	62.472	-2.768	71.212	1.00	23.60
ATOM	5240	O	PHE	B	279	61.866	-3.697	70.678	1.00	26.54
ATOM	5241	N	ASN	B	280	63.677	-2.376	70.804	1.00	21.93
ATOM	5242	CA	ASN	B	280	64.318	-3.046	69.680	1.00	23.70
ATOM	5243	CB	ASN	B	280	65.520	-2.248	69.164	1.00	22.63
ATOM	5244	CG	ASN	B	280	65.107	-0.937	68.505	1.00	30.83
ATOM	5245	OD1	ASN	B	280	64.094	-0.878	67.796	1.00	25.81
ATOM	5246	ND2	ASN	B	280	65.900	0.112	68.714	1.00	26.54
ATOM	5247	C	ASN	B	280	64.746	-4.466	70.009	1.00	26.10
ATOM	5248	O	ASN	B	280	64.775	-5.321	69.124	1.00	26.16
ATOM	5249	N	ILE	B	281	65.080	-4.724	71.272	1.00	26.10
ATOM	5250	CA	ILE	B	281	65.485	-6.067	71.667	1.00	25.81
ATOM	5251	CB	ILE	B	281	66.006	-6.098	73.124	1.00	28.50
ATOM	5252	CG2	ILE	B	281	66.046	-7.527	73.648	1.00	28.53
ATOM	5253	CG1	ILE	B	281	67.392	-5.454	73.173	1.00	32.07
ATOM	5254	CD1	ILE	B	281	68.038	-5.442	74.541	1.00	28.24
ATOM	5255	C	ILE	B	281	64.320	-7.030	71.507	1.00	25.77
ATOM	5256	O	ILE	B	281	64.484	-8.131	70.982	1.00	23.39
ATOM	5257	N	VAL	B	282	63.139	-6.618	71.950	1.00	21.30
ATOM	5258	CA	VAL	B	282	61.961	-7.465	71.813	1.00	22.90
ATOM	5259	CB	VAL	B	282	60.703	-6.775	72.387	1.00	24.07
ATOM	5260	CG1	VAL	B	282	59.464	-7.611	72.093	1.00	22.28
ATOM	5261	CG2	VAL	B	282	60.865	-6.587	73.906	1.00	26.89
ATOM	5262	C	VAL	B	282	61.718	-7.795	70.339	1.00	23.87
ATOM	5263	O	VAL	B	282	61.462	-8.949	69.978	1.00	22.65
ATOM	5264	N	ARG	B	283	61.799	-6.779	69.488	1.00	23.19
ATOM	5265	CA	ARG	B	283	61.576	-6.971	68.060	1.00	27.95
ATOM	5266	CB	ARG	B	283	61.510	-5.612	67.359	1.00	25.48
ATOM	5267	CG	ARG	B	283	60.337	-4.760	67.838	1.00	26.55
ATOM	5268	CD	ARG	B	283	60.442	-3.333	67.339	1.00	31.52
ATOM	5269	NE	ARG	B	283	60.210	-3.208	65.908	1.00	24.43
ATOM	5270	CZ	ARG	B	283	60.915	-2.414	65.116	1.00	26.45
ATOM	5271	NH1	ARG	B	283	61.902	-1.676	65.622	1.00	26.04
ATOM	5272	NH2	ARG	B	283	60.634	-2.356	63.825	1.00	29.64
ATOM	5273	C	ARG	B	283	62.634	-7.855	67.402	1.00	32.04
ATOM	5274	O	ARG	B	283	62.341	-8.552	66.431	1.00	29.76
ATOM	5275	N	GLU	B	284	63.859	-7.821	67.923	1.00	31.50
ATOM	5276	CA	GLU	B	284	64.934	-8.646	67.381	1.00	32.42
ATOM	5277	CB	GLU	B	284	66.289	-8.260	67.992	1.00	38.31
ATOM	5278	CG	GLU	B	284	66.798	-6.864	67.640	1.00	48.93
ATOM	5279	CD	GLU	B	284	68.102	-6.518	68.362	1.00	56.28
ATOM	5280	OE1	GLU	B	284	69.084	-7.281	68.222	1.00	57.37
ATOM	5281	OE2	GLU	B	284	68.150	-5.485	69.069	1.00	55.42
ATOM	5282	C	GLU	B	284	64.638	-10.105	67.714	1.00	31.93
ATOM	5283	O	GLU	B	284	64.899	-11.001	66.913	1.00	28.26
ATOM	5284	N	VAL	B	285	64.089	-10.340	68.901	1.00	28.09
ATOM	5285	CA	VAL	B	285	63.765	-11.697	69.325	1.00	30.67
ATOM	5286	CB	VAL	B	285	63.687	-11.802	70.863	1.00	28.33
ATOM	5287	CG1	VAL	B	285	63.257	-13.206	71.262	1.00	29.84
ATOM	5288	CG2	VAL	B	285	65.037	-11.470	71.478	1.00	26.93
ATOM	5289	C	VAL	B	285	62.460	-12.265	68.758	1.00	31.19
ATOM	5290	O	VAL	B	285	62.422	-13.423	68.349	1.00	31.38
ATOM	5291	N	PHE	B	286	61.398	-11.460	68.729	1.00	28.21
ATOM	5292	CA	PHE	B	286	60.105	-11.948	68.249	1.00	25.71
ATOM	5293	CB	PHE	B	286	59.064	-11.853	69.374	1.00	24.57
ATOM	5294	CG	PHE	B	286	59.311	-12.804	70.514	1.00	26.87
ATOM	5295	CD1	PHE	B	286	59.651	-12.331	71.779	1.00	25.16
ATOM	5296	CD2	PHE	B	286	59.205	-14.180	70.319	1.00	22.51
ATOM	5297	CE1	PHE	B	286	59.880	-13.213	72.833	1.00	22.92
ATOM	5298	CE2	PHE	B	286	59.433	-15.063	71.362	1.00	21.99
ATOM	5299	CZ	PHE	B	286	59.772	-14.578	72.626	1.00	26.75
ATOM	5300	C	PHE	B	286	59.518	-11.318	66.993	1.00	25.90
ATOM	5301	O	PHE	B	286	58.388	-11.630	66.620	1.00	22.84
ATOM	5302	N	GLY	B	287	60.272	-10.451	66.329	1.00	28.27
ATOM	5303	CA	GLY	B	287	59.756	-9.814	65.130	1.00	23.38

ATOM	5304	C	GLY	B	287	58.765	-8.719	65.498	1.00	29.17
ATOM	5305	O	GLY	B	287	58.786	-8.216	56.517	1.00	22.88
ATOM	5306	N	GLU	B	288	57.896	-8.361	64.558	1.00	26.77
ATOM	5307	CA	GLU	B	288	56.893	-7.324	64.754	1.00	25.38
ATOM	5308	CB	GLU	B	288	56.405	-6.791	63.405	1.00	29.51
ATOM	5309	CG	GLU	B	288	57.430	-6.003	62.605	1.00	36.06
ATOM	5310	CD	GLU	B	288	57.906	-4.769	63.347	1.00	41.10
ATOM	5311	OE1	GLU	B	288	57.058	-4.055	63.919	1.00	41.19
ATOM	5312	OE2	GLU	B	288	59.125	-4.503	63.348	1.00	44.69
ATOM	5313	C	GLU	B	288	55.682	-7.819	65.527	1.00	27.87
ATOM	5314	O	GLU	B	288	55.209	-8.931	65.308	1.00	26.80
ATOM	5315	N	GLY	B	289	55.176	-6.973	66.419	1.00	24.53
ATOM	5316	CA	GLY	B	289	54.006	-7.326	67.204	1.00	29.17
ATOM	5317	C	GLY	B	289	53.015	-6.171	67.244	1.00	30.46
ATOM	5318	O	GLY	B	289	53.005	-5.326	66.358	1.00	26.17
ATOM	5319	N	VAL	B	290	52.171	-6.142	68.268	1.00	23.95
ATOM	5320	CA	VAL	B	290	51.194	-5.079	68.440	1.00	22.25
ATOM	5321	CB	VAL	B	290	49.794	-5.655	68.783	1.00	18.71
ATOM	5322	CG1	VAL	B	290	48.810	-4.525	69.047	1.00	22.67
ATOM	5323	CG2	VAL	B	290	49.289	-6.504	67.629	1.00	19.26
ATOM	5324	C	VAL	B	290	51.722	-4.232	69.593	1.00	21.55
ATOM	5325	O	VAL	B	290	51.960	-4.741	70.687	1.00	21.32
ATOM	5326	N	TYR	B	291	51.913	-2.941	69.346	1.00	21.06
ATOM	5327	CA	TYR	B	291	52.479	-2.063	70.357	1.00	19.29
ATOM	5328	CB	TYR	B	291	53.582	-1.216	69.711	1.00	20.40
ATOM	5329	CG	TYR	B	291	54.553	-2.072	68.918	1.00	23.09
ATOM	5330	CD1	TYR	B	291	54.740	-1.875	67.549	1.00	19.52
ATOM	5331	CE1	TYR	B	291	55.580	-2.712	66.809	1.00	20.67
ATOM	5332	CD2	TYR	B	291	55.234	-3.122	69.527	1.00	22.88
ATOM	5333	CE2	TYR	B	291	56.070	-3.960	68.800	1.00	26.04
ATOM	5334	CZ	TYR	B	291	56.235	-3.752	67.442	1.00	23.44
ATOM	5335	OH	TYR	B	291	57.027	-4.612	66.722	1.00	28.02
ATOM	5336	C	TYR	B	291	51.465	-1.180	71.068	1.00	26.89
ATOM	5337	O	TYR	B	291	50.668	-0.479	70.429	1.00	20.26
ATOM	5338	N	LEU	B	292	51.522	-1.204	72.399	1.00	21.75
ATOM	5339	CA	LEU	B	292	50.604	-0.426	73.227	1.00	22.11
ATOM	5340	CB	LEU	B	292	49.765	-1.369	74.088	1.00	20.92
ATOM	5341	CG	LEU	B	292	49.091	-2.542	73.375	1.00	22.94
ATOM	5342	CD1	LEU	B	292	48.328	-3.362	74.411	1.00	21.03
ATOM	5343	CD2	LEU	B	292	48.149	-2.043	72.281	1.00	18.04
ATOM	5344	C	LEU	B	292	51.330	0.557	74.147	1.00	21.59
ATOM	5345	O	LEU	B	292	52.514	0.404	74.426	1.00	19.96
ATOM	5346	N	GLY	B	293	50.606	1.571	74.613	1.00	23.31
ATOM	5347	CA	GLY	B	293	51.195	2.537	75.521	1.00	20.76
ATOM	5348	C	GLY	B	293	51.163	1.979	76.930	1.00	26.15
ATOM	5349	O	GLY	B	293	51.263	0.765	77.133	1.00	20.96
ATOM	5350	N	GLY	B	294	51.017	2.859	77.914	1.00	24.63
ATOM	5351	CA	GLY	B	294	50.980	2.407	79.293	1.00	20.00
ATOM	5352	C	GLY	B	294	51.176	3.538	80.285	1.00	22.59
ATOM	5353	O	GLY	B	294	51.145	4.719	79.916	1.00	17.46
ATOM	5354	N	GLY	B	295	51.373	3.179	81.551	1.00	17.10
ATOM	5355	CA	GLY	B	295	51.577	4.180	82.582	1.00	16.52
ATOM	5356	C	GLY	B	295	52.695	5.145	82.232	1.00	19.54
ATOM	5357	O	GLY	B	295	53.738	4.737	81.732	1.00	16.31
ATOM	5358	N	GLY	B	296	52.467	6.430	82.497	1.00	21.93
ATOM	5359	CA	GLY	B	296	53.448	7.465	82.207	1.00	20.05
ATOM	5360	C	GLY	B	296	52.869	8.750	82.759	1.00	22.20
ATOM	5361	O	GLY	B	296	51.790	9.160	82.336	1.00	20.48
ATOM	5362	N	TYR	B	297	53.573	9.402	83.682	1.00	20.93
ATOM	5363	CA	TYR	B	297	53.025	10.598	84.306	1.00	23.25
ATOM	5364	CB	TYR	B	297	52.731	10.284	85.774	1.00	19.93
ATOM	5365	CG	TYR	B	297	52.041	8.944	85.900	1.00	24.76
ATOM	5366	CD1	TYR	B	297	52.779	7.758	85.936	1.00	21.97
ATOM	5367	CE1	TYR	B	297	52.148	6.514	85.912	1.00	19.79
ATOM	5368	CD2	TYR	B	297	50.653	8.850	85.849	1.00	20.86
ATOM	5369	CE2	TYR	B	297	50.012	7.612	85.822	1.00	19.57

Figure 18-82

ATOM	5370	CZ	TYR	B	297	50.758	6.457	85.851	1.00	23.85
ATOM	5371	OH	TYR	B	297	50.106	5.254	85.806	1.00	17.83
ATOM	5372	C	TYR	B	297	53.839	11.877	84.181	1.00	25.22
ATOM	5373	O	TYR	B	297	53.451	12.925	84.705	1.00	21.77
ATOM	5374	N	HIS	B	298	54.974	11.794	83.497	1.00	23.21
ATOM	5375	CA	HIS	B	298	55.787	12.976	83.270	1.00	25.62
ATOM	5376	CB	HIS	B	298	57.270	12.713	83.534	1.00	22.88
ATOM	5377	CG	HIS	B	298	58.097	13.956	83.502	1.00	25.13
ATOM	5378	CD2	HIS	B	298	58.406	14.791	82.482	1.00	28.22
ATOM	5379	ND1	HIS	B	298	58.617	14.536	84.641	1.00	32.76
ATOM	5380	CE1	HIS	B	298	59.209	15.674	84.323	1.00	26.52
ATOM	5381	NE2	HIS	B	298	59.094	15.852	83.019	1.00	32.15
ATOM	5382	C	HIS	B	298	55.589	13.307	81.795	1.00	25.66
ATOM	5383	O	HIS	B	298	56.087	12.589	80.923	1.00	25.84
ATOM	5384	N	PRO	B	299	54.901	14.424	81.496	1.00	27.02
ATOM	5385	CD	PRO	B	299	54.388	15.424	82.447	1.00	29.91
ATOM	5386	CA	PRO	B	299	54.616	14.864	80.127	1.00	26.53
ATOM	5387	CB	PRO	B	299	53.952	16.232	80.342	1.00	27.76
ATOM	5388	CG	PRO	B	299	54.583	16.696	81.656	1.00	27.97
ATOM	5389	C	PRO	B	299	55.815	14.930	79.194	1.00	27.08
ATOM	5390	O	PRO	B	299	55.738	14.472	78.057	1.00	28.58
ATOM	5391	N	TYR	B	300	56.925	15.484	79.668	1.00	27.30
ATOM	5392	CA	TYR	B	300	58.114	15.593	78.824	1.00	27.17
ATOM	5393	CB	TYR	B	300	59.173	16.496	79.466	1.00	31.65
ATOM	5394	CG	TYR	B	300	58.684	17.851	79.921	1.00	31.61
ATOM	5395	CD1	TYR	B	300	57.414	18.318	79.582	1.00	32.71
ATOM	5396	CE1	TYR	B	300	56.971	19.568	80.014	1.00	38.52
ATOM	5397	CD2	TYR	B	300	59.499	18.670	80.701	1.00	30.92
ATOM	5398	CE2	TYR	B	300	59.072	19.917	81.138	1.00	32.13
ATOM	5399	CZ	TYR	B	300	57.808	20.361	80.795	1.00	39.17
ATOM	5400	OH	TYR	B	300	57.374	21.585	81.252	1.00	43.90
ATOM	5401	C	TYR	B	300	58.731	14.218	78.572	1.00	25.20
ATOM	5402	O	TYR	B	300	59.106	13.894	77.445	1.00	25.15
ATOM	5403	N	ALA	B	301	58.845	13.419	79.628	1.00	20.55
ATOM	5404	CA	ALA	B	301	59.414	12.080	79.508	1.00	22.12
ATOM	5405	CB	ALA	B	301	59.417	11.388	80.874	1.00	17.09
ATOM	5406	C	ALA	B	301	58.608	11.260	78.505	1.00	15.20
ATOM	5407	O	ALA	B	301	59.161	10.629	77.613	1.00	17.12
ATOM	5408	N	LEU	B	302	57.295	11.290	78.667	1.00	18.02
ATOM	5409	CA	LEU	B	302	56.381	10.553	77.815	1.00	19.88
ATOM	5410	CB	LEU	B	302	54.957	10.702	78.362	1.00	21.72
ATOM	5411	CG	LEU	B	302	53.767	10.118	77.606	1.00	31.08
ATOM	5412	CD1	LEU	B	302	52.576	9.980	78.549	1.00	31.35
ATOM	5413	CD2	LEU	B	302	53.434	11.011	76.415	1.00	27.11
ATOM	5414	C	LEU	B	302	56.445	10.988	76.351	1.00	21.13
ATOM	5415	O	LEU	B	302	56.473	10.149	75.449	1.00	21.76
ATOM	5416	N	ALA	B	303	56.472	12.293	76.115	1.00	17.69
ATOM	5417	CA	ALA	B	303	56.516	12.811	74.755	1.00	17.79
ATOM	5418	CB	ALA	B	303	56.357	14.326	74.780	1.00	24.50
ATOM	5419	C	ALA	B	303	57.803	12.425	74.040	1.00	20.84
ATOM	5420	O	ALA	B	303	57.781	11.968	72.891	1.00	19.33
ATOM	5421	N	ARG	B	304	58.930	12.594	74.723	1.00	21.08
ATOM	5422	CA	ARG	B	304	60.215	12.269	74.120	1.00	25.56
ATOM	5423	CB	ARG	B	304	61.375	12.825	74.962	1.00	18.37
ATOM	5424	CG	ARG	B	304	61.427	14.356	75.072	1.00	23.12
ATOM	5425	CD	ARG	B	304	62.797	14.758	75.624	1.00	29.00
ATOM	5426	NE	ARG	B	304	63.073	13.938	76.789	1.00	33.28
ATOM	5427	CZ	ARG	B	304	64.271	13.689	77.283	1.00	30.24
ATOM	5428	NH1	ARG	B	304	65.363	14.194	76.723	1.00	24.98
ATOM	5429	NH2	ARG	B	304	64.365	12.896	78.333	1.00	36.15
ATOM	5430	C	ARG	B	304	60.406	10.775	73.922	1.00	20.46
ATOM	5431	O	ARG	B	304	60.850	10.338	72.868	1.00	18.70
ATOM	5432	N	ALA	B	305	60.070	9.988	74.937	1.00	22.48
ATOM	5433	CA	ALA	B	305	60.226	8.542	74.845	1.00	19.70
ATOM	5434	CB	ALA	B	305	59.847	7.894	76.174	1.00	24.24
ATOM	5435	C	ALA	B	305	59.407	7.930	73.711	1.00	15.82

Figure 18-83

ATOM	5436	O	ALA	B	305	59.938	7.184	72.888	1.00	19.12
ATOM	5437	N	TRP	B	306	58.113	8.230	73.659	1.00	18.65
ATOM	5438	CA	TRP	B	306	57.298	7.668	72.600	1.00	19.57
ATOM	5439	CB	TRP	B	306	55.800	7.856	72.893	1.00	18.26
ATOM	5440	CG	TRP	B	306	55.301	6.911	73.953	1.00	20.71
ATOM	5441	CD2	TRP	B	306	54.087	7.025	74.708	1.00	23.94
ATOM	5442	CE2	TRP	B	306	53.988	5.870	75.513	1.00	24.73
ATOM	5443	CE3	TRP	B	306	53.073	7.991	74.780	1.00	26.01
ATOM	5444	CD1	TRP	B	306	55.872	5.721	74.326	1.00	20.04
ATOM	5445	NE1	TRP	B	306	55.092	5.093	75.260	1.00	19.17
ATOM	5446	CZ2	TRP	B	306	52.912	5.655	76.385	1.00	28.04
ATOM	5447	CZ3	TRP	B	306	52.001	7.779	75.646	1.00	28.68
ATOM	5448	CH2	TRP	B	306	51.930	6.619	76.437	1.00	31.22
ATOM	5449	C	TRP	B	306	57.665	8.223	71.226	1.00	23.48
ATOM	5450	O	TRP	B	306	57.416	7.574	70.212	1.00	22.38
ATOM	5451	N	THR	B	307	58.262	9.412	71.176	1.00	22.36
ATOM	5452	CA	THR	B	307	58.672	9.953	69.880	1.00	25.94
ATOM	5453	CB	THR	B	307	59.143	11.417	69.986	1.00	25.88
ATOM	5454	OG1	THR	B	307	58.015	12.261	70.258	1.00	21.07
ATOM	5455	CG2	THR	B	307	59.827	11.864	68.686	1.00	22.52
ATOM	5456	C	THR	B	307	59.815	9.078	69.350	1.00	30.09
ATOM	5457	O	THR	B	307	59.922	8.834	68.144	1.00	25.82
ATOM	5458	N	LEU	B	308	60.664	8.596	70.258	1.00	27.54
ATOM	5459	CA	LEU	B	308	61.773	7.734	69.857	1.00	26.76
ATOM	5460	CB	LEU	B	308	62.691	7.424	71.054	1.00	24.24
ATOM	5461	CG	LEU	B	308	63.420	8.614	71.718	1.00	31.16
ATOM	5462	CD1	LEU	B	308	64.282	8.147	72.877	1.00	24.71
ATOM	5463	CD2	LEU	B	308	64.289	9.325	70.700	1.00	24.59
ATOM	5464	C	LEU	B	308	61.184	6.443	69.287	1.00	27.20
ATOM	5465	O	LEU	B	308	61.609	5.961	68.234	1.00	23.52
ATOM	5466	N	ILE	B	309	60.190	5.898	69.980	1.00	25.10
ATOM	5467	CA	ILE	B	309	59.537	4.679	69.530	1.00	25.14
ATOM	5468	CB	ILE	B	309	58.387	4.266	70.485	1.00	27.05
ATOM	5469	CG2	ILE	B	309	57.646	3.058	69.926	1.00	23.57
ATOM	5470	CG1	ILE	B	309	58.952	3.947	71.868	1.00	22.98
ATOM	5471	CD1	ILE	B	309	59.927	2.793	71.868	1.00	24.25
ATOM	5472	C	ILE	B	309	58.958	4.885	68.133	1.00	25.41
ATOM	5473	O	ILE	B	309	59.177	4.064	67.243	1.00	22.13
ATOM	5474	N	TRP	B	310	58.232	5.984	67.943	1.00	27.45
ATOM	5475	CA	TRP	B	310	57.618	6.266	66.648	1.00	29.27
ATOM	5476	CB	TRP	B	310	56.721	7.505	66.715	1.00	27.00
ATOM	5477	CG	TRP	B	310	56.112	7.847	65.378	1.00	28.26
ATOM	5478	CD2	TRP	B	310	55.172	7.061	64.633	1.00	27.50
ATOM	5479	CE2	TRP	B	310	54.947	7.729	63.408	1.00	30.47
ATOM	5480	CE3	TRP	B	310	54.500	5.856	64.877	1.00	29.85
ATOM	5481	CD1	TRP	B	310	56.406	9.929	64.597	1.00	29.76
ATOM	5482	NE1	TRP	B	310	55.713	8.865	63.415	1.00	26.71
ATOM	5483	CZ2	TRP	B	310	54.076	8.234	62.429	1.00	28.23
ATOM	5484	CZ3	TRP	B	310	53.636	5.362	63.901	1.00	30.24
ATOM	5485	CH2	TRP	B	310	53.433	6.053	62.692	1.00	27.63
ATOM	5486	C	TRP	B	310	58.629	6.424	65.520	1.00	30.16
ATOM	5487	O	TRP	B	310	58.378	5.964	64.410	1.00	30.04
ATOM	5488	N	CYS	B	311	59.762	7.069	65.793	1.00	24.26
ATOM	5489	CA	CYS	B	311	60.782	7.233	64.764	1.00	27.97
ATOM	5490	CB	CYS	B	311	61.893	8.157	65.252	1.00	28.21
ATOM	5491	SG	CYS	B	311	61.422	9.905	65.381	1.00	33.38
ATOM	5492	C	CYS	B	311	61.380	5.886	64.351	1.00	30.02
ATOM	5493	O	CYS	B	311	61.670	5.660	63.172	1.00	25.45
ATOM	5494	N	GLU	B	312	61.570	5.001	65.327	1.00	31.59
ATOM	5495	CA	GLU	B	312	62.111	3.669	65.067	1.00	33.48
ATOM	5496	CB	GLU	B	312	62.142	2.843	66.352	1.00	34.78
ATOM	5497	CG	GLU	B	312	63.487	2.307	66.758	1.00	39.45
ATOM	5498	CD	GLU	B	312	64.171	1.513	65.675	1.00	40.11
ATOM	5499	OE1	GLU	B	312	63.539	0.614	65.081	1.00	43.69
ATOM	5500	OE2	GLU	B	312	65.358	1.782	65.437	1.00	39.26
ATOM	5501	C	GLU	B	312	61.197	2.959	64.080	1.00	29.97

ATOM	5502	O	GLU B 312	61.640	2.497	63.035	1.00	31.38
ATOM	5503	N	LEU B 313	59.919	2.865	64.438	1.00	26.70
ATOM	5504	CA	LEU B 313	58.930	2.203	63.598	1.00	26.73
ATOM	5505	CB	LEU B 313	57.571	2.173	64.297	1.00	25.83
ATOM	5506	CG	LEU B 313	57.429	1.224	65.477	1.00	35.18
ATOM	5507	CD1	LEU B 313	56.063	1.434	66.130	1.00	32.49
ATOM	5508	CD2	LEU B 313	57.595	-0.215	64.989	1.00	29.71
ATOM	5509	C	LEU B 313	58.768	2.866	62.248	1.00	29.03
ATOM	5510	O	LEU B 313	58.716	2.187	61.228	1.00	25.39
ATOM	5511	N	SER B 314	58.677	4.194	62.263	1.00	30.13
ATOM	5512	CA	SER B 314	58.498	5.006	61.060	1.00	34.06
ATOM	5513	CB	SER B 314	58.206	6.456	61.445	1.00	31.15
ATOM	5514	OG	SER B 314	57.041	6.537	62.234	1.00	48.58
ATOM	5515	C	SER B 314	59.707	5.003	60.151	1.00	31.84
ATOM	5516	O	SER B 314	59.632	5.469	59.026	1.00	34.15
ATOM	5517	N	GLY B 315	60.831	4.515	60.655	1.00	31.81
ATOM	5518	CA	GLY B 315	62.036	4.485	59.848	1.00	37.27
ATOM	5519	C	GLY B 315	62.659	5.851	59.616	1.00	39.93
ATOM	5520	O	GLY B 315	63.363	6.054	58.624	1.00	39.79
ATOM	5521	N	ARG B 316	62.422	6.798	60.518	1.00	38.22
ATOM	5522	CA	ARG B 316	63.004	8.121	60.336	1.00	38.66
ATOM	5523	CB	ARG B 316	61.908	9.184	60.275	1.00	40.20
ATOM	5524	CG	ARG B 316	61.089	9.345	61.520	1.00	39.00
ATOM	5525	CD	ARG B 316	60.032	10.398	61.284	1.00	42.13
ATOM	5526	NE	ARG B 316	59.002	9.954	60.352	1.00	45.09
ATOM	5527	CZ	ARG B 316	58.075	10.754	59.838	1.00	40.84
ATOM	5528	NH1	ARG B 316	58.064	12.033	60.170	1.00	48.44
ATOM	5529	NH2	ARG B 316	57.150	10.278	59.014	1.00	35.96
ATOM	5530	C	ARG B 316	64.031	8.467	61.408	1.00	39.03
ATOM	5531	O	ARG B 316	63.952	7.988	62.539	1.00	34.34
ATOM	5532	N	GLU B 317	65.003	9.296	61.035	1.00	39.58
ATOM	5533	CA	GLU B 317	66.074	9.697	61.943	1.00	43.35
ATOM	5534	CB	GLU B 317	67.142	10.509	61.203	1.00	49.34
ATOM	5535	CG	GLU B 317	67.609	9.910	59.884	1.00	57.04
ATOM	5536	CD	GLU B 317	66.546	10.009	58.798	1.00	62.79
ATOM	5537	OE1	GLU B 317	66.146	11.149	58.467	1.00	63.46
ATOM	5538	OE2	GLU B 317	66.108	8.954	58.280	1.00	64.46
ATOM	5539	C	GLU B 317	65.555	10.528	63.100	1.00	41.58
ATOM	5540	O	GLU B 317	64.658	11.356	62.939	1.00	39.74
ATOM	5541	N	VAL B 318	66.118	10.301	64.278	1.00	35.38
ATOM	5542	CA	VAL B 318	65.706	11.049	65.448	1.00	38.76
ATOM	5543	CB	VAL B 318	66.000	10.265	66.750	1.00	42.28
ATOM	5544	CG1	VAL B 318	65.560	11.080	67.962	1.00	38.26
ATOM	5545	CG2	VAL B 318	65.287	8.916	66.722	1.00	39.99
ATOM	5546	C	VAL B 318	66.459	12.370	65.478	1.00	41.82
ATOM	5547	O	VAL B 318	67.689	12.395	65.570	1.00	37.20
ATOM	5548	N	PRO B 319	65.735	13.491	65.356	1.00	43.18
ATOM	5549	CD	PRO B 319	64.290	13.672	65.155	1.00	41.90
ATOM	5550	CA	PRO B 319	66.402	14.792	65.388	1.00	44.31
ATOM	5551	CB	PRO B 319	65.241	15.763	65.181	1.00	44.58
ATOM	5552	CG	PRO B 319	64.079	15.011	65.795	1.00	43.34
ATOM	5553	C	PRO B 319	67.086	14.965	66.741	1.00	44.62
ATOM	5554	O	PRO B 319	66.541	14.565	67.771	1.00	43.75
ATOM	5555	N	GLU B 320	68.277	15.552	66.735	1.00	44.16
ATOM	5556	CA	GLU B 320	69.029	15.762	67.967	1.00	45.92
ATOM	5557	CB	GLU B 320	70.381	16.406	67.663	1.00	50.87
ATOM	5558	CG	GLU B 320	71.165	16.768	68.919	1.00	53.71
ATOM	5559	CD	GLU B 320	72.455	17.505	68.620	1.00	57.75
ATOM	5560	OE1	GLU B 320	73.161	17.874	69.583	1.00	56.37
ATOM	5561	OE2	GLU B 320	72.762	17.714	67.427	1.00	60.07
ATOM	5562	C	GLU B 320	68.311	16.625	68.995	1.00	44.42
ATOM	5563	O	GLU B 320	68.244	16.279	70.168	1.00	42.32
ATOM	5564	N	LYS B 321	67.778	17.753	68.550	1.00	42.50
ATOM	5565	CA	LYS B 321	67.102	18.672	69.448	1.00	45.24
ATOM	5566	CB	LYS B 321	67.853	20.000	69.503	1.00	46.43
ATOM	5567	CG	LYS B 321	67.890	20.802	68.195	1.00	51.45

Figure 18-85

ATOM	5568	CD	LYS	B	321	68.700	20.144	67.057	1.00	57.24
ATOM	5569	CE	LYS	B	321	67.936	19.062	66.280	1.00	55.24
ATOM	5570	NZ	LYS	B	321	66.738	19.588	65.558	1.00	55.31
ATOM	5571	C	LYS	B	321	65.662	18.971	69.098	1.00	43.44
ATOM	5572	O	LYS	B	321	65.211	18.736	67.978	1.00	43.03
ATOM	5573	N	LEU	B	322	64.947	19.512	70.076	1.00	39.45
ATOM	5574	CA	LEU	B	322	63.563	19.885	69.875	1.00	40.31
ATOM	5575	CB	LEU	B	322	62.846	20.034	71.215	1.00	40.88
ATOM	5576	CG	LEU	B	322	62.943	18.901	72.234	1.00	40.09
ATOM	5577	CD1	LEU	B	322	62.001	19.175	73.388	1.00	38.17
ATOM	5578	CD2	LEU	B	322	62.588	17.596	71.580	1.00	41.56
ATOM	5579	C	LEU	B	322	63.615	21.244	69.197	1.00	41.23
ATOM	5580	O	LEU	B	322	64.466	22.070	69.531	1.00	39.22
ATOM	5581	N	ASN	B	323	62.735	21.473	68.233	1.00	40.04
ATOM	5582	CA	ASN	B	323	62.703	22.771	67.582	1.00	43.32
ATOM	5583	CB	ASN	B	323	61.985	22.707	66.234	1.00	41.53
ATOM	5584	CG	ASN	B	323	60.617	22.085	66.335	1.00	41.89
ATOM	5585	OD1	ASN	B	323	59.889	22.308	67.304	1.00	39.79
ATOM	5586	ND2	ASN	B	323	60.243	21.317	65.317	1.00	40.43
ATOM	5587	C	ASN	B	323	61.949	23.690	68.532	1.00	44.76
ATOM	5588	O	ASN	B	323	61.402	23.237	69.539	1.00	45.80
ATOM	5589	N	ASN	B	324	61.902	24.973	68.210	1.00	46.85
ATOM	5590	CA	ASN	B	324	61.234	25.930	69.076	1.00	47.60
ATOM	5591	CB	ASN	B	324	61.460	27.348	68.549	1.00	50.87
ATOM	5592	CG	ASN	B	324	61.089	28.407	69.562	1.00	55.06
ATOM	5593	OD1	ASN	B	324	59.925	28.565	69.919	1.00	60.68
ATOM	5594	ND2	ASN	B	324	62.091	29.131	70.048	1.00	59.17
ATOM	5595	C	ASN	B	324	59.740	25.664	69.249	1.00	43.97
ATOM	5596	O	ASN	B	324	59.190	25.898	70.322	1.00	41.33
ATOM	5597	N	LYS	B	325	59.087	25.168	68.201	1.00	43.49
ATOM	5598	CA	LYS	B	325	57.655	24.892	68.264	1.00	45.95
ATOM	5599	CB	LYS	B	325	57.112	24.415	66.909	1.00	48.97
ATOM	5600	CG	LYS	B	325	57.212	25.400	65.731	1.00	53.41
ATOM	5601	CD	LYS	B	325	58.582	25.386	65.024	1.00	58.77
ATOM	5602	CE	LYS	B	325	59.700	26.013	65.846	1.00	58.10
ATOM	5603	NZ	LYS	B	325	61.024	25.906	65.178	1.00	53.38
ATOM	5604	C	LYS	B	325	57.368	23.822	69.309	1.00	45.79
ATOM	5605	O	LYS	B	325	56.375	23.891	70.034	1.00	43.91
ATOM	5606	N	ALA	B	326	58.245	22.829	69.381	1.00	44.28
ATOM	5607	CA	ALA	B	326	58.078	21.746	70.336	1.00	44.25
ATOM	5608	CB	ALA	B	326	59.013	20.589	69.986	1.00	41.44
ATOM	5609	C	ALA	B	326	58.342	22.233	71.757	1.00	40.92
ATOM	5610	O	ALA	B	326	57.639	21.843	72.688	1.00	39.02
ATOM	5611	N	LYS	B	327	59.352	23.085	71.922	1.00	38.14
ATOM	5612	CA	LYS	B	327	59.689	23.603	73.246	1.00	40.11
ATOM	5613	CB	LYS	B	327	60.892	24.552	73.178	1.00	42.36
ATOM	5614	CG	LYS	B	327	62.174	23.922	72.159	1.00	45.78
ATOM	5615	CD	LYS	B	327	63.325	24.926	72.675	1.00	48.46
ATOM	5616	CE	LYS	B	327	64.594	24.367	72.031	1.00	49.62
ATOM	5617	NZ	LYS	B	327	65.108	23.139	72.700	1.00	48.53
ATOM	5618	C	LYS	B	327	58.500	24.338	73.841	1.00	39.17
ATOM	5619	O	LYS	B	327	58.132	24.112	74.994	1.00	38.87
ATOM	5620	N	GLU	B	328	57.898	25.215	73.048	1.00	41.06
ATOM	5621	CA	GLU	B	328	56.750	25.986	73.512	1.00	42.35
ATOM	5622	CB	GLU	B	328	56.357	27.028	72.463	1.00	44.02
ATOM	5623	CG	GLU	B	328	57.434	28.084	72.258	1.00	44.80
ATOM	5624	CD	GLU	B	328	57.835	28.742	73.569	1.00	48.40
ATOM	5625	OE1	GLU	B	328	56.949	29.317	74.237	1.00	51.20
ATOM	5626	OE2	GLU	B	328	59.029	28.680	73.935	1.00	47.81
ATOM	5627	C	GLU	B	328	55.569	25.087	73.839	1.00	38.67
ATOM	5628	O	GLU	B	328	54.794	25.377	74.750	1.00	41.20
ATOM	5629	N	LEU	B	329	55.429	23.999	73.090	1.00	35.31
ATOM	5630	CA	LEU	B	329	54.349	23.056	73.334	1.00	32.69
ATOM	5631	CB	LEU	B	329	54.404	21.900	72.334	1.00	35.06
ATOM	5632	CG	LEU	B	329	53.344	20.813	72.544	1.00	35.01
ATOM	5633	CD1	LEU	B	329	51.958	21.430	72.419	1.00	36.90

ATOM	5634	CD2	LEU	B	329	53.521	19.699	71.525	1.00	32.36
ATOM	5635	C	LEU	B	329	54.504	22.507	74.747	1.00	34.07
ATOM	5636	O	LEU	B	329	53.621	22.664	75.583	1.00	30.53
ATOM	5637	N	LEU	B	330	55.640	21.873	75.013	1.00	32.74
ATOM	5638	CA	LEU	B	330	55.889	21.311	76.330	1.00	34.99
ATOM	5639	CB	LEU	B	330	57.267	20.642	76.382	1.00	37.01
ATOM	5640	CG	LEU	B	330	57.466	19.428	75.470	1.00	34.91
ATOM	5641	CD1	LEU	B	330	58.832	18.817	75.728	1.00	34.69
ATOM	5642	CD2	LEU	B	330	56.369	18.396	75.742	1.00	34.10
ATOM	5643	C	LEU	B	330	55.789	22.363	77.429	1.00	37.12
ATOM	5644	O	LEU	B	330	55.210	22.110	78.482	1.00	34.19
ATOM	5645	N	LYS	B	331	56.353	23.540	77.186	1.00	34.34
ATOM	5646	CA	LYS	B	331	56.313	24.604	78.181	1.00	43.35
ATOM	5647	CB	LYS	B	331	57.162	25.788	77.712	1.00	46.25
ATOM	5648	CG	LYS	B	331	58.658	25.496	77.685	1.00	51.07
ATOM	5649	CD	LYS	B	331	59.482	26.610	77.021	1.00	49.96
ATOM	5650	CE	LYS	B	331	59.371	27.957	77.733	1.00	53.08
ATOM	5651	NZ	LYS	B	331	58.013	28.569	77.662	1.00	56.18
ATOM	5652	C	LYS	B	331	54.892	25.069	78.494	1.00	42.06
ATOM	5653	O	LYS	B	331	54.588	25.416	79.631	1.00	43.05
ATOM	5654	N	SER	B	332	54.018	25.056	77.492	1.00	44.54
ATOM	5655	CA	SER	B	332	52.639	25.502	77.679	1.00	46.58
ATOM	5656	CB	SER	B	332	51.975	25.751	76.329	1.00	48.75
ATOM	5657	OG	SER	B	332	51.769	24.527	75.646	1.00	49.55
ATOM	5658	C	SER	B	332	51.780	24.507	78.451	1.00	49.56
ATOM	5659	O	SER	B	332	50.618	24.791	78.749	1.00	46.67
ATOM	5660	N	ILE	B	333	52.341	23.345	78.770	1.00	50.55
ATOM	5661	CA	ILE	B	333	51.586	22.326	79.488	1.00	51.93
ATOM	5662	CB	ILE	B	333	52.259	20.945	79.376	1.00	51.82
ATOM	5663	CG2	ILE	B	333	51.447	19.902	80.134	1.00	50.29
ATOM	5664	CG1	ILE	B	333	52.359	20.539	77.905	1.00	52.18
ATOM	5665	CD1	ILE	B	333	53.044	19.210	77.693	1.00	55.42
ATOM	5666	C	ILE	B	333	51.367	22.634	80.964	1.00	51.45
ATOM	5667	O	ILE	B	333	52.180	23.290	81.614	1.00	50.96
ATOM	5668	N	ASP	B	334	50.245	22.141	81.472	1.00	54.05
ATOM	5669	CA	ASP	B	334	49.850	22.306	82.865	1.00	58.15
ATOM	5670	CB	ASP	B	334	48.320	22.216	82.959	1.00	60.38
ATOM	5671	CG	ASP	B	334	47.751	20.972	82.262	1.00	63.85
ATOM	5672	GD1	ASP	B	334	48.017	19.833	82.710	1.00	59.16
ATOM	5673	OD2	ASP	B	334	47.033	21.138	81.252	1.00	59.71
ATOM	5674	C	ASP	B	334	50.506	21.207	83.701	1.00	55.47
ATOM	5675	O	ASP	B	334	49.833	20.291	84.171	1.00	54.08
ATOM	5676	N	PHE	B	335	51.816	21.307	83.906	1.00	54.60
ATOM	5677	CA	PHE	B	335	52.524	20.266	84.641	1.00	56.60
ATOM	5678	CB	PHE	B	335	53.718	19.784	83.811	1.00	53.01
ATOM	5679	CG	PHE	B	335	54.522	18.717	84.482	1.00	49.30
ATOM	5680	CD1	PHE	B	335	53.898	17.589	85.008	1.00	45.61
ATOM	5681	CD2	PHE	B	335	55.901	18.843	84.605	1.00	46.83
ATOM	5682	CE1	PHE	B	335	54.637	16.600	85.651	1.00	45.95
ATOM	5683	CE2	PHE	B	335	56.651	17.860	85.247	1.00	46.02
ATOM	5684	CZ	PHE	B	335	56.018	16.737	85.772	1.00	46.08
ATOM	5685	C	PHE	B	335	52.971	20.559	86.072	1.00	57.29
ATOM	5686	O	PHE	B	335	52.197	20.378	87.012	1.00	63.54
ATOM	5687	N	GLU	B	336	54.223	20.983	86.229	1.00	55.21
ATOM	5688	CA	GLU	B	336	54.818	21.286	87.535	1.00	60.30
ATOM	5689	CB	GLU	B	336	53.783	21.846	88.517	1.00	64.95
ATOM	5690	CG	GLU	B	336	54.375	22.225	89.867	1.00	71.50
ATOM	5691	CD	GLU	B	336	53.363	22.882	90.787	1.00	75.37
ATOM	5692	OE1	GLU	B	336	52.796	23.925	90.394	1.00	75.32
ATOM	5693	OE2	GLU	B	336	53.137	22.361	91.901	1.00	76.84
ATOM	5694	C	GLU	B	336	55.485	20.058	88.146	1.00	55.66
ATOM	5695	O	GLU	B	336	54.823	19.093	88.529	1.00	49.97
ATOM	5696	N	GLU	B	337	56.807	20.125	88.240	1.00	54.26
ATOM	5697	CA	GLU	B	337	57.630	19.047	88.767	1.00	54.35
ATOM	5698	CB	GLU	B	337	59.101	19.457	88.635	1.00	54.08
ATOM	5699	CG	GLU	B	337	60.074	18.315	88.514	1.00	54.15

ATOM	5700	CD	GLU	B	337	59.856	17.496	87.259	1.00	48.94
ATOM	5701	OE1	GLU	B	337	59.958	18.049	86.142	1.00	41.06
ATOM	5702	OE2	GLU	B	337	59.581	16.292	87.391	1.00	50.23
ATOM	5703	C	GLU	B	337	57.278	18.740	90.227	1.00	55.08
ATOM	5704	O	GLU	B	337	57.130	19.651	91.039	1.00	54.51
ATOM	5705	N	PHE	B	338	57.140	17.458	90.557	1.00	56.20
ATOM	5706	CA	PHE	B	338	56.798	17.048	91.918	1.00	57.73
ATOM	5707	CB	PHE	B	338	56.713	15.527	92.020	1.00	58.47
ATOM	5708	CG	PHE	B	338	56.231	15.034	93.359	1.00	63.17
ATOM	5709	CD1	PHE	B	338	54.882	15.096	93.696	1.00	64.86
ATOM	5710	CD2	PHE	B	338	57.129	14.526	94.293	1.00	63.51
ATOM	5711	CE1	PHE	B	338	54.434	14.656	94.943	1.00	65.25
ATOM	5712	CE2	PHE	B	338	56.693	14.087	95.539	1.00	63.64
ATOM	5713	CZ	PHE	B	338	55.342	14.152	95.864	1.00	66.30
ATOM	5714	C	PHE	B	338	57.836	17.539	92.918	1.00	61.85
ATOM	5715	O	PHE	B	338	57.520	17.807	94.078	1.00	58.15
ATOM	5716	N	ASP	B	339	59.081	17.636	92.466	1.00	64.63
ATOM	5717	CA	ASP	B	339	60.167	18.099	93.316	1.00	67.53
ATOM	5718	CB	ASP	B	339	61.286	17.059	93.362	1.00	67.32
ATOM	5719	CG	ASP	B	339	62.474	17.524	94.174	1.00	68.13
ATOM	5720	OD1	ASP	B	339	62.280	17.909	95.346	1.00	68.68
ATOM	5721	OD2	ASP	B	339	63.603	17.502	93.646	1.00	69.03
ATOM	5722	C	ASP	B	339	60.718	19.435	92.829	1.00	69.03
ATOM	5723	O	ASP	B	339	61.211	19.545	91.708	1.00	67.54
ATOM	5724	N	ASP	B	340	60.626	20.442	93.693	1.00	72.19
ATOM	5725	CA	ASP	B	340	61.088	21.797	93.402	1.00	75.20
ATOM	5726	CB	ASP	B	340	61.113	22.623	94.689	1.00	77.04
ATOM	5727	CG	ASP	B	340	59.766	22.671	95.375	1.00	78.70
ATOM	5728	OD1	ASP	B	340	58.803	23.181	94.763	1.00	79.66
ATOM	5729	OD2	ASP	B	340	59.668	22.194	96.525	1.00	80.53
ATOM	5730	C	ASP	B	340	62.464	21.856	92.751	1.00	74.82
ATOM	5731	O	ASP	B	340	62.615	22.400	91.659	1.00	78.48
ATOM	5732	N	GLU	B	341	63.465	21.303	93.426	1.00	74.11
ATOM	5733	CA	GLU	B	341	64.827	21.312	92.907	1.00	76.25
ATOM	5734	CB	GLU	B	341	65.818	21.596	94.040	1.00	79.54
ATOM	5735	CG	GLU	B	341	67.277	21.653	93.596	1.00	82.33
ATOM	5736	CD	GLU	B	341	67.539	22.750	92.577	1.00	83.24
ATOM	5737	OE1	GLU	B	341	67.333	23.937	92.910	1.00	85.25
ATOM	5738	OE2	GLU	B	341	67.950	22.427	91.443	1.00	83.72
ATOM	5739	C	GLU	B	341	65.196	19.998	92.227	1.00	73.97
ATOM	5740	O	GLU	B	341	65.627	19.051	92.883	1.00	77.10
ATOM	5741	N	VAL	B	342	65.033	19.946	90.910	1.00	71.92
ATOM	5742	CA	VAL	B	342	65.354	18.744	90.151	1.00	68.51
ATOM	5743	CB	VAL	B	342	64.081	18.027	89.663	1.00	68.83
ATOM	5744	CG1	VAL	B	342	63.268	17.552	90.837	1.00	67.57
ATOM	5745	CG2	VAL	B	342	63.255	18.969	88.806	1.00	67.72
ATOM	5746	C	VAL	B	342	66.201	19.059	88.927	1.00	65.35
ATOM	5747	O	VAL	B	342	67.177	18.366	88.640	1.00	68.21
ATOM	5748	N	ASP	B	343	65.819	20.112	88.213	1.00	60.89
ATOM	5749	CA	ASP	B	343	66.514	20.520	86.998	1.00	58.89
ATOM	5750	CB	ASP	B	343	68.024	20.636	87.223	1.00	63.48
ATOM	5751	CG	ASP	B	343	68.763	21.070	85.966	1.00	66.69
ATOM	5752	OD1	ASP	B	343	70.012	21.070	85.970	1.00	67.64
ATOM	5753	OD2	ASP	B	343	68.089	21.420	84.973	1.00	65.42
ATOM	5754	C	ASP	B	343	66.264	19.499	85.900	1.00	53.17
ATOM	5755	O	ASP	B	343	66.993	18.516	85.766	1.00	49.70
ATOM	5756	N	ARG	B	344	65.216	19.735	85.124	1.00	50.24
ATOM	5757	CA	ARG	B	344	64.868	18.853	84.022	1.00	46.49
ATOM	5758	CB	ARG	B	344	63.467	18.269	84.228	1.00	42.41
ATOM	5759	CG	ARG	B	344	63.317	17.367	85.452	1.00	38.59
ATOM	5760	CD	ARG	B	344	64.344	16.246	85.432	1.00	37.12
ATOM	5761	NE	ARG	B	344	64.169	15.310	86.537	1.00	36.55
ATOM	5762	CZ	ARG	B	344	65.078	14.413	86.905	1.00	37.20
ATOM	5763	NH1	ARG	B	344	66.234	14.331	86.259	1.00	33.53
ATOM	5764	NH2	ARG	B	344	64.830	13.595	87.915	1.00	28.79
ATOM	5765	C	ARG	B	344	64.910	19.660	82.732	1.00	44.45

Figure 18-88

ATOM	5766	O	ARG	B	344	64.328	19.269	81.720	1.00	38.73
ATOM	5767	N	SER	B	345	65.618	20.784	82.783	1.00	42.44
ATOM	5768	CA	SER	B	345	65.740	21.677	81.637	1.00	41.74
ATOM	5769	CB	SER	B	345	66.661	22.849	81.993	1.00	43.47
ATOM	5770	OG	SER	B	345	67.956	22.388	82.351	1.00	46.96
ATOM	5771	C	SER	B	345	66.244	20.981	80.375	1.00	36.32
ATOM	5772	O	SER	B	345	65.840	21.333	79.273	1.00	35.70
ATOM	5773	N	TYR	B	346	67.117	19.992	80.534	1.00	33.93
ATOM	5774	CA	TYR	B	346	67.661	19.264	79.391	1.00	34.77
ATOM	5775	CB	TYR	B	346	68.660	18.206	79.877	1.00	36.09
ATOM	5776	CG	TYR	B	346	68.054	17.146	80.774	1.00	34.27
ATOM	5777	CD1	TYR	B	346	67.433	16.013	80.240	1.00	37.62
ATOM	5778	CE1	TYR	B	346	66.843	15.048	81.077	1.00	36.73
ATOM	5779	CD2	TYR	B	346	68.072	17.294	82.157	1.00	36.40
ATOM	5780	CE2	TYR	B	346	67.489	16.344	82.999	1.00	36.54
ATOM	5781	CZ	TYR	B	346	66.878	15.228	82.457	1.00	36.54
ATOM	5782	OH	TYR	B	346	66.310	14.306	83.306	1.00	33.35
ATOM	5783	C	TYR	B	346	66.563	18.599	78.570	1.00	36.26
ATOM	5784	O	TYR	B	346	66.719	18.385	77.367	1.00	40.50
ATOM	5785	N	MET	B	347	65.445	18.282	79.214	1.00	32.72
ATOM	5786	CA	MET	B	347	64.346	17.628	78.516	1.00	35.43
ATOM	5787	CB	MET	B	347	63.280	17.164	79.513	1.00	34.36
ATOM	5788	CG	MET	B	347	63.819	16.292	80.635	1.00	28.32
ATOM	5789	SD	MET	B	347	62.515	15.604	81.669	1.00	34.47
ATOM	5790	CE	MET	B	347	61.654	17.027	82.142	1.00	39.60
ATOM	5791	C	MET	B	347	63.701	18.525	77.465	1.00	39.04
ATOM	5792	O	MET	B	347	63.060	18.029	76.540	1.00	37.38
ATOM	5793	N	LEU	B	348	63.857	19.839	77.606	1.00	39.21
ATOM	5794	CA	LEU	B	348	63.272	20.773	76.645	1.00	40.81
ATOM	5795	CB	LEU	B	348	62.806	22.058	77.339	1.00	36.87
ATOM	5796	CG	LEU	B	348	61.690	21.975	78.384	1.00	42.66
ATOM	5797	CD1	LEU	B	348	61.507	23.337	79.032	1.00	43.41
ATOM	5798	CD2	LEU	B	348	60.391	21.511	77.741	1.00	40.47
ATOM	5799	C	LEU	B	348	64.289	21.133	75.573	1.00	41.13
ATOM	5800	O	LEU	B	348	64.018	21.968	74.711	1.00	38.93
ATOM	5801	N	GLU	B	349	65.455	20.495	75.632	1.00	37.70
ATOM	5802	CA	GLU	B	349	66.527	20.757	74.681	1.00	42.48
ATOM	5803	CB	GLU	B	349	67.856	20.953	75.422	1.00	45.02
ATOM	5804	CG	GLU	B	349	67.834	22.035	76.493	1.00	53.82
ATOM	5805	CD	GLU	B	349	67.483	23.402	75.938	1.00	57.46
ATOM	5806	OE1	GLU	B	349	68.211	23.885	75.044	1.00	59.62
ATOM	5807	OE2	GLU	B	349	66.480	23.993	76.397	1.00	57.91
ATOM	5808	C	GLU	B	349	66.709	19.638	73.664	1.00	43.57
ATOM	5809	O	GLU	B	349	66.577	19.849	72.459	1.00	41.26
ATOM	5810	N	THR	B	350	67.027	18.448	74.161	1.00	41.95
ATOM	5811	CA	THR	B	350	67.264	17.299	73.298	1.00	40.02
ATOM	5812	CB	THR	B	350	68.689	16.775	73.504	1.00	43.08
ATOM	5813	OG1	THR	B	350	68.894	16.490	74.894	1.00	41.07
ATOM	5814	CG2	THR	B	350	69.703	17.816	73.049	1.00	45.05
ATOM	5815	C	THR	B	350	66.278	16.154	73.510	1.00	37.56
ATOM	5816	O	THR	B	350	65.754	15.966	74.611	1.00	33.64
ATOM	5817	N	LEU	B	351	66.043	15.391	72.445	1.00	32.86
ATOM	5818	CA	LEU	B	351	65.126	14.260	72.475	1.00	35.00
ATOM	5819	CB	LEU	B	351	64.776	13.810	71.053	1.00	31.61
ATOM	5820	CG	LEU	B	351	63.709	14.601	70.312	1.00	35.31
ATOM	5821	CD1	LEU	B	351	63.552	14.064	68.904	1.00	37.88
ATOM	5822	CD2	LEU	B	351	62.397	14.474	71.068	1.00	39.36
ATOM	5823	C	LEU	B	351	65.662	13.065	73.240	1.00	33.33
ATOM	5824	O	LEU	B	351	64.956	12.469	74.046	1.00	31.48
ATOM	5825	N	LYS	B	352	66.915	12.720	72.981	1.00	29.58
ATOM	5826	CA	LYS	B	352	67.527	11.576	73.633	1.00	36.77
ATOM	5827	CB	LYS	B	352	68.457	10.864	72.647	1.00	34.32
ATOM	5828	CG	LYS	B	352	67.777	10.563	71.326	1.00	39.29
ATOM	5829	CD	LYS	B	352	68.703	9.949	70.294	1.00	42.25
ATOM	5830	CE	LYS	B	352	69.110	8.541	70.655	1.00	46.22
ATOM	5831	NZ	LYS	B	352	69.831	7.905	69.516	1.00	44.15

205/263

Figure 18-89

ATOM	5832	C	LYS	B	352	68.295	11.983	74.878	1.00	36.20
ATOM	5833	O	LYS	B	352	69.086	12.931	74.865	1.00	36.65
ATOM	5834	N	ASP	B	353	68.049	11.275	75.967	1.00	30.01
ATOM	5835	CA	ASP	B	353	68.757	11.569	77.188	1.00	33.99
ATOM	5836	CB	ASP	B	353	67.852	11.308	78.394	1.00	38.57
ATOM	5837	CG	ASP	B	353	67.134	9.986	78.315	1.00	43.90
ATOM	5838	OD1	ASP	B	353	66.034	9.851	78.926	1.00	22.39
ATOM	5839	OD2	ASP	B	353	67.679	9.078	77.649	1.00	50.42
ATOM	5840	C	ASP	B	353	70.022	10.723	77.202	1.00	35.83
ATOM	5841	O	ASP	B	353	70.189	9.833	76.368	1.00	23.71
ATOM	5842	N	PRO	B	354	70.954	11.025	78.116	1.00	36.36
ATOM	5843	CD	PRO	B	354	70.928	12.093	79.132	1.00	38.28
ATOM	5844	CA	PRO	B	354	72.205	10.277	78.212	1.00	33.62
ATOM	5845	CB	PRO	B	354	73.003	11.104	79.213	1.00	34.46
ATOM	5846	CG	PRO	B	354	71.896	11.556	80.164	1.00	38.08
ATOM	5847	C	PRO	B	354	71.924	8.883	78.733	1.00	33.62
ATOM	5848	O	PRO	B	354	70.894	8.643	79.366	1.00	24.82
ATOM	5849	N	TRP	B	355	72.833	7.954	78.468	1.00	31.76
ATOM	5850	CA	TRP	B	355	72.635	6.611	78.969	1.00	30.01
ATOM	5851	CB	TRP	B	355	73.653	5.655	78.359	1.00	34.02
ATOM	5852	CG	TRP	B	355	73.025	4.378	77.910	1.00	44.37
ATOM	5853	CD2	TRP	B	355	73.263	3.072	78.436	1.00	45.39
ATOM	5854	CE2	TRP	B	355	72.418	2.177	77.734	1.00	44.31
ATOM	5855	CE3	TRP	B	355	74.107	2.569	79.432	1.00	47.19
ATOM	5856	CD1	TRP	B	355	72.073	4.230	76.935	1.00	42.18
ATOM	5857	NE1	TRP	B	355	71.704	2.910	76.826	1.00	37.84
ATOM	5858	C22	TRP	B	355	72.395	0.808	77.999	1.00	44.97
ATOM	5859	CZ3	TRP	B	355	74.084	1.207	79.694	1.00	50.83
ATOM	5860	CH2	TRP	B	355	73.231	0.341	78.979	1.00	48.73
ATOM	5861	C	TRP	B	355	72.819	6.685	80.485	1.00	30.67
ATOM	5862	O	TRP	B	355	73.622	7.474	80.981	1.00	26.93
ATOM	5863	N	ARG	B	356	72.061	5.880	81.218	1.00	24.96
ATOM	5864	CA	ARG	B	356	72.147	5.848	82.671	1.00	23.57
ATOM	5865	CB	ARG	B	356	70.811	6.319	83.257	1.00	24.71
ATOM	5866	CG	ARG	B	356	70.534	7.795	82.941	1.00	23.66
ATOM	5867	CD	ARG	B	356	69.067	8.212	83.055	1.00	20.14
ATOM	5868	NE	ARG	B	356	68.926	9.610	82.642	1.00	20.59
ATOM	5869	CZ	ARG	B	356	67.787	10.192	82.288	1.00	25.41
ATOM	5870	NH1	ARG	B	356	66.644	9.508	82.287	1.00	17.01
ATOM	5871	NH2	ARG	B	356	67.796	11.464	81.910	1.00	20.07
ATOM	5872	C	ARG	B	356	72.481	4.410	83.085	1.00	26.57
ATOM	5873	O	ARG	B	356	71.610	3.641	83.485	1.00	23.02
ATOM	5874	N	GLY	B	357	73.761	4.063	82.978	1.00	23.92
ATOM	5875	CA	GLY	B	357	74.186	2.712	83.294	1.00	25.54
ATOM	5876	C	GLY	B	357	74.796	2.464	84.657	1.00	24.35
ATOM	5877	O	GLY	B	357	74.523	3.161	85.628	1.00	25.88
ATOM	5878	N	GLY	B	358	75.638	1.444	84.718	1.00	24.32
ATOM	5879	CA	GLY	B	358	76.282	1.070	85.960	1.00	23.56
ATOM	5880	C	GLY	B	358	76.412	-0.441	85.924	1.00	29.26
ATOM	5881	O	GLY	B	358	76.146	-1.051	84.889	1.00	23.71
ATOM	5882	N	GLU	B	359	76.814	-1.051	87.033	1.00	27.64
ATOM	5883	CA	GLU	B	359	76.955	-2.503	87.078	1.00	32.16
ATOM	5884	CB	GLU	B	359	77.822	-2.936	88.265	1.00	30.40
ATOM	5885	CG	GLU	B	359	77.125	-2.772	89.601	1.00	31.23
ATOM	5886	CD	GLU	B	359	77.844	-3.479	90.741	1.00	37.96
ATOM	5887	OE1	GLU	B	359	77.287	-3.521	91.861	1.00	33.89
ATOM	5888	OE2	GLU	B	359	78.959	-3.990	90.520	1.00	37.40
ATOM	5889	C	GLU	B	359	75.571	-3.122	87.261	1.00	31.35
ATOM	5890	O	GLU	B	359	74.612	-2.429	87.588	1.00	25.15
ATOM	5891	N	VAL	B	360	75.482	-4.428	87.053	1.00	29.61
ATOM	5892	CA	VAL	B	360	74.230	-5.147	87.251	1.00	26.21
ATOM	5893	CB	VAL	B	360	74.035	-6.270	86.200	1.00	28.47
ATOM	5894	CG1	VAL	B	360	72.764	-7.045	86.492	1.00	22.74
ATOM	5895	CG2	VAL	B	360	73.969	-5.670	84.796	1.00	29.70
ATOM	5896	C	VAL	B	360	74.342	-5.784	88.625	1.00	26.00
ATOM	5897	O	VAL	B	360	75.150	-6.693	88.821	1.00	27.55

ATOM	5898	N	ARG B 361	73.553	-5.289	89.575	1.00	26.45
ATOM	5899	CA	ARG B 361	73.558	-5.921	90.935	1.00	28.47
ATOM	5900	CB	ARG B 361	72.479	-5.146	91.787	1.00	30.55
ATOM	5901	CG	ARG B 361	72.937	-3.877	92.485	1.00	32.61
ATOM	5902	CD	ARG B 361	71.749	-3.163	93.117	1.00	35.00
ATOM	5903	NE	ARG B 361	70.858	-2.617	92.094	1.00	30.31
ATOM	5904	CZ	ARG B 361	69.753	-1.925	92.350	1.00	29.45
ATOM	5905	NH1	ARG B 361	69.385	-1.689	93.605	1.00	18.49
ATOM	5906	NH2	ARG B 361	69.041	-1.428	91.348	1.00	30.49
ATOM	5907	C	ARG B 361	73.351	-7.322	91.001	1.00	30.17
ATOM	5908	O	ARG B 361	72.665	-7.910	90.168	1.00	23.60
ATOM	5909	N	LYS B 362	73.949	-7.922	92.022	1.00	33.09
ATOM	5910	CA	LYS B 362	73.864	-9.351	92.272	1.00	36.94
ATOM	5911	CB	LYS B 362	74.687	-9.706	93.513	1.00	40.24
ATOM	5912	CG	LYS B 362	76.190	-9.527	93.337	1.00	52.55
ATOM	5913	CD	LYS B 362	76.571	-8.126	92.849	1.00	56.65
ATOM	5914	CE	LYS B 362	76.149	-7.032	93.819	1.00	53.39
ATOM	5915	NZ	LYS B 362	76.553	-5.680	93.341	1.00	48.87
ATOM	5916	C	LYS B 362	72.427	-9.826	92.463	1.00	32.84
ATOM	5917	O	LYS B 362	72.045	-10.867	91.938	1.00	28.27
ATOM	5918	N	GLU B 363	71.628	-9.075	93.215	1.00	34.67
ATOM	5919	CA	GLU B 363	70.245	-9.493	93.435	1.00	35.72
ATOM	5920	CB	GLU B 363	69.519	-8.532	94.390	1.00	36.04
ATOM	5921	CG	GLU B 363	69.502	-7.077	93.977	1.00	44.81
ATOM	5922	CD	GLU B 363	68.859	-6.186	95.033	1.00	52.14
ATOM	5923	OE1	GLU B 363	67.661	-6.370	95.341	1.00	48.46
ATOM	5924	OE2	GLU B 363	69.562	-5.300	95.566	1.00	57.31
ATOM	5925	C	GLU B 363	69.501	-9.619	92.111	1.00	30.68
ATOM	5926	O	GLU B 363	68.695	-10.530	91.944	1.00	30.45
ATOM	5927	N	VAL B 364	69.784	-8.724	91.166	1.00	26.19
ATOM	5928	CA	VAL B 364	69.138	-8.789	89.852	1.00	24.65
ATOM	5929	CB	VAL B 364	69.536	-7.599	88.958	1.00	23.49
ATOM	5930	CG1	VAL B 364	68.924	-7.770	87.563	1.00	21.01
ATOM	5931	CG2	VAL B 364	69.049	-6.293	89.587	1.00	23.08
ATOM	5932	C	VAL B 364	69.530	-10.083	89.144	1.00	23.19
ATOM	5933	O	VAL B 364	68.691	-10.749	88.542	1.00	23.06
ATOM	5934	N	LYS B 365	70.810	-10.436	89.216	1.00	27.15
ATOM	5935	CA	LYS B 365	71.296	-11.668	88.594	1.00	29.18
ATOM	5936	CB	LYS B 365	72.821	-11.758	88.704	1.00	28.61
ATOM	5937	CG	LYS B 365	73.554	-10.617	88.030	1.00	30.27
ATOM	5938	CD	LYS B 365	75.074	-10.768	88.154	1.00	32.58
ATOM	5939	CE	LYS B 365	75.790	-9.587	87.516	1.00	29.13
ATOM	5940	NZ	LYS B 365	77.271	-9.689	87.606	1.00	35.17
ATOM	5941	C	LYS B 365	70.666	-12.879	89.276	1.00	25.30
ATOM	5942	O	LYS B 365	70.282	-13.837	88.613	1.00	26.81
ATOM	5943	N	ASP B 366	70.559	-12.831	90.604	1.00	26.10
ATOM	5944	CA	ASP B 366	69.963	-13.938	91.347	1.00	28.29
ATOM	5945	CB	ASP B 366	70.105	-13.731	92.859	1.00	29.44
ATOM	5946	CG	ASP B 366	71.557	-13.669	93.311	1.00	32.95
ATOM	5947	OD1	ASP B 366	72.446	-14.099	92.551	1.00	26.37
ATOM	5948	OD2	ASP B 366	71.811	-13.216	94.442	1.00	35.26
ATOM	5949	C	ASP B 366	68.487	-14.110	90.986	1.00	28.61
ATOM	5950	O	ASP B 366	68.000	-15.231	90.869	1.00	27.00
ATOM	5951	N	THR B 367	67.777	-13.002	90.801	1.00	28.63
ATOM	5952	CA	THR B 367	66.365	-13.080	90.438	1.00	27.35
ATOM	5953	CB	THR B 367	65.726	-11.683	90.359	1.00	27.63
ATOM	5954	OG1	THR B 367	65.771	-11.068	91.656	1.00	28.12
ATOM	5955	CG2	THR B 367	64.280	-11.786	89.890	1.00	22.94
ATOM	5956	C	THR B 367	66.197	-13.782	89.094	1.00	25.46
ATOM	5957	O	THR B 367	65.389	-14.693	88.964	1.00	24.48
ATOM	5958	N	LEU B 368	66.962	-13.361	88.092	1.00	23.33
ATOM	5959	CA	LEU B 368	66.857	-13.990	86.785	1.00	28.99
ATOM	5960	CB	LEU B 368	67.719	-13.256	85.759	1.00	27.67
ATOM	5961	CG	LEU B 368	67.060	-12.070	85.046	1.00	29.47
ATOM	5962	CD1	LEU B 368	65.923	-12.607	84.195	1.00	32.45
ATOM	5963	CD2	LEU B 368	66.546	-11.027	86.043	1.00	19.43

207/263

Figure 18-91

ATOM	5964	C	LEU	B	368	67.262	-15.454	86.888	1.00	32.40
ATOM	5965	O	LEU	B	368	66.726	-16.309	86.179	1.00	31.80
ATOM	5966	N	GLU	B	369	68.212	-15.735	87.774	1.00	33.59
ATOM	5967	CA	GLU	B	369	68.656	-17.101	88.003	1.00	39.68
ATOM	5968	CB	GLU	B	369	69.736	-17.141	89.082	1.00	42.61
ATOM	5969	CG	GLU	B	369	71.133	-17.138	88.537	1.00	50.65
ATOM	5970	CD	GLU	B	369	71.469	-18.443	87.842	1.00	55.81
ATOM	5971	OE1	GLU	B	369	72.589	-18.561	87.299	1.00	57.42
ATOM	5972	OE2	GLU	B	369	70.610	-19.353	87.841	1.00	58.37
ATOM	5973	C	GLU	B	369	67.479	-17.954	88.442	1.00	34.94
ATOM	5974	O	GLU	B	369	67.190	-18.974	87.827	1.00	32.71
ATOM	5975	N	LYS	B	370	66.805	-17.541	89.512	1.00	34.92
ATOM	5976	CA	LYS	B	370	65.656	-18.295	89.993	1.00	35.12
ATOM	5977	CB	LYS	B	370	65.061	-17.679	91.268	1.00	37.39
ATOM	5978	CG	LYS	B	370	65.879	-17.916	92.532	1.00	44.70
ATOM	5979	CD	LYS	B	370	66.781	-16.741	92.892	1.00	48.10
ATOM	5980	CE	LYS	B	370	65.956	-15.537	93.346	1.00	47.82
ATOM	5981	NZ	LYS	B	370	66.804	-14.387	93.786	1.00	45.41
ATOM	5982	C	LYS	B	370	64.581	-18.375	88.930	1.00	33.21
ATOM	5983	O	LYS	B	370	63.937	-19.409	88.773	1.00	29.52
ATOM	5984	N	ALA	B	371	64.390	-17.288	88.191	1.00	31.62
ATOM	5985	CA	ALA	B	371	63.368	-17.274	87.153	1.00	37.19
ATOM	5986	CB	ALA	B	371	63.392	-15.938	86.403	1.00	35.65
ATOM	5987	C	ALA	B	371	63.572	-18.431	86.181	1.00	37.79
ATOM	5988	O	ALA	B	371	62.627	-19.137	85.838	1.00	34.46
ATOM	5989	N	LYS	B	372	64.810	-18.644	85.759	1.00	40.10
ATOM	5990	CA	LYS	B	372	65.147	-19.698	84.792	1.00	40.46
ATOM	5991	C	LYS	B	372	64.746	-21.066	85.348	1.00	43.15
ATOM	5992	O	LYS	B	372	64.757	-22.053	84.591	1.00	43.57
ATOM	5993	CB	LYS	B	372	66.654	-19.694	84.517	1.00	40.51
ATOM	5994	CG	LYS	B	372	67.029	-18.925	83.248	1.00	20.00
ATOM	5995	CD	LYS	B	372	68.352	-19.390	82.635	1.00	20.00
ATOM	5996	CE	LYS	B	372	68.544	-20.907	82.706	1.00	20.00
ATOM	5997	NZ	LYS	B	372	69.814	-21.354	82.116	1.00	20.00
ATOM	5998	N	ALA	B	373	64.412	-21.159	86.624	1.00	47.80
ATOM	5999	CA	ALA	B	373	64.014	-22.425	87.239	1.00	49.71
ATOM	6000	CB	ALA	B	373	64.762	-22.639	88.546	1.00	48.25
ATOM	6001	C	ALA	B	373	62.515	-22.443	87.494	1.00	53.38
ATOM	6002	O	ALA	B	373	61.844	-23.313	86.903	1.00	58.01
ATOM	6003	OXT	ALA	B	373	62.029	-21.589	88.269	1.00	55.13
HETATM	2991	ZN	ZN	C	1	49.660	9.211	109.302	1.00	32.54
HETATM	2992	O1	TSA	D	2	47.669	8.189	109.464	1.00	28.76
HETATM	2993	O2	TSA	D	2	49.952	6.981	108.340	1.00	25.81
HETATM	2994	O3	TSA	D	2	52.458	5.101	101.667	1.00	36.93
HETATM	2995	N1	TSA	D	2	47.800	7.789	108.131	1.00	31.21
HETATM	2996	N2	TSA	D	2	53.013	-1.329	101.259	1.00	30.57
HETATM	2997	C1	TSA	D	2	51.859	2.799	101.610	1.00	28.47
HETATM	2998	C2	TSA	D	2	50.907	1.769	101.666	1.00	25.57
HETATM	2999	C3	TSA	D	2	51.241	0.419	101.551	1.00	21.68
HETATM	3000	C4	TSA	D	2	52.626	0.026	101.366	1.00	23.11
HETATM	3001	C5	TSA	D	2	53.589	1.080	101.303	1.00	25.02
HETATM	3002	C6	TSA	D	2	53.218	2.408	101.418	1.00	29.24
HETATM	3003	C7	TSA	D	2	51.572	4.261	101.734	1.00	32.98
HETATM	3004	C8	TSA	D	2	50.108	4.726	101.996	1.00	29.05
HETATM	3005	C9	TSA	D	2	50.052	5.421	103.338	1.00	28.13
HETATM	3006	C10	TSA	D	2	49.060	5.357	104.279	1.00	25.99
HETATM	3007	C11	TSA	D	2	49.315	6.155	105.504	1.00	32.05
HETATM	3008	C12	TSA	D	2	48.515	6.184	106.595	1.00	27.37
HETATM	3009	C13	TSA	D	2	48.855	6.994	107.756	1.00	29.02
HETATM	3010	C14	TSA	D	2	49.680	5.693	100.864	1.00	30.21
HETATM	3011	C15	TSA	D	2	47.776	4.545	104.132	1.00	30.60
HETATM	3012	C17	TSA	D	2	54.438	-1.703	101.139	1.00	23.45
HETATM	3013	C16	TSA	D	2	52.044	-2.416	101.316	1.00	23.15
HETATM	6004	ZN	ZN	E	1	52.949	1.842	85.681	1.00	28.19
HETATM	6005	O1	TSA	F	2	50.964	0.911	85.428	1.00	24.72
HETATM	6006	O2	TSA	F	2	51.255	3.324	86.654	1.00	30.24

208/263

Figure 18-92

HETATM	6007	O3	TSA	F	2	51.569	6.512	93.219	1.00	27.89
HETATM	6008	N1	TSA	F	2	50.347	1.221	86.634	1.00	27.23
HETATM	6009	N2	TSA	F	2	47.061	11.139	93.713	1.00	16.24
HETATM	6010	C1	TSA	F	2	49.443	7.579	93.304	1.00	27.18
HETATM	6011	C2	TSA	F	2	48.035	7.529	93.267	1.00	25.98
HETATM	6012	C3	TSA	F	2	47.227	8.657	93.398	1.00	24.59
HETATM	6013	C4	TSA	F	2	47.837	9.971	93.583	1.00	25.75
HETATM	6014	C5	TSA	F	2	49.274	10.017	93.626	1.00	26.53
HETATM	6015	C6	TSA	F	2	50.041	8.869	93.495	1.00	28.36
HETATM	6016	C7	TSA	F	2	50.349	6.405	93.167	1.00	25.27
HETATM	6017	C8	TSA	F	2	49.716	5.006	92.905	1.00	24.18
HETATM	6018	C9	TSA	F	2	50.134	4.552	91.518	1.00	27.20
HETATM	6019	C10	TSA	F	2	49.419	3.807	90.616	1.00	30.21
HETATM	6020	C11	TSA	F	2	50.118	3.553	89.327	1.00	27.18
HETATM	6021	C12	TSA	F	2	49.762	2.624	88.409	1.00	23.47
HETATM	6022	C13	TSA	F	2	50.529	2.462	87.170	1.00	28.28
HETATM	6023	C14	TSA	F	2	50.208	4.019	93.994	1.00	28.83
HETATM	6024	C15	TSA	F	2	48.013	3.270	90.863	1.00	26.16
HETATM	6025	C17	TSA	F	2	47.699	12.456	93.883	1.00	27.37
HETATM	6026	C16	TSA	F	2	45.610	11.107	93.679	1.00	25.36
HETATM	6027	OH2	WAT	G	1	61.391	6.723	88.062	1.00	12.93
HETATM	6028	OH2	WAT	G	2	55.595	-4.443	83.558	1.00	7.53
HETATM	6029	OH2	WAT	G	3	58.656	12.731	106.749	1.00	12.33
HETATM	6030	OH2	WAT	G	4	46.347	15.263	111.460	1.00	14.54
HETATM	6031	OH2	WAT	G	5	45.523	13.627	76.224	1.00	11.14
HETATM	6032	OH2	WAT	G	6	24.466	-6.064	85.688	1.00	22.41
HETATM	6033	OH2	WAT	G	7	48.579	-17.745	80.769	1.00	21.99
HETATM	6034	OH2	WAT	G	8	56.344	-15.640	87.809	1.00	26.67
HETATM	6035	OH2	WAT	G	9	48.554	-14.901	83.717	1.00	23.94
HETATM	6036	OH2	WAT	G	10	57.540	-7.620	122.771	1.00	26.96
HETATM	6037	OH2	WAT	G	11	59.414	-2.497	84.029	1.00	22.51
HETATM	6038	OH2	WAT	G	12	31.671	18.074	114.616	1.00	32.15
HETATM	6039	OH2	WAT	G	13	62.335	10.679	117.140	1.00	19.47
HETATM	6040	OH2	WAT	G	14	45.565	9.469	79.366	1.00	18.81
HETATM	6041	OH2	WAT	G	15	43.311	8.237	79.508	1.00	26.11
HETATM	6042	OH2	WAT	G	16	46.628	13.883	104.423	1.00	24.28
HETATM	6043	OH2	WAT	G	17	40.672	2.507	81.576	1.00	18.30
HETATM	6044	OH2	WAT	G	18	61.830	10.923	77.709	1.00	22.27
HETATM	6045	OH2	WAT	G	19	57.813	0.831	108.580	1.00	24.68
HETATM	6046	OH2	WAT	G	20	48.885	5.660	77.823	1.00	30.00
HETATM	6047	OH2	WAT	G	21	36.382	-8.352	88.841	1.00	17.32
HETATM	6048	OH2	WAT	G	22	39.316	-10.091	86.422	1.00	27.38
HETATM	6049	OH2	WAT	G	23	54.802	-3.446	90.346	1.00	21.73
HETATM	6050	OH2	WAT	G	24	49.292	12.112	140.537	1.00	34.17
HETATM	6051	OH2	WAT	G	25	56.747	8.830	60.744	1.00	40.67
HETATM	6052	OH2	WAT	G	26	41.952	9.79	100.118	1.00	27.92
HETATM	6053	OH2	WAT	G	27	31.268	2.80	106.695	1.00	24.31
HETATM	6054	OH2	WAT	G	28	68.342	17.79	111.076	1.00	30.93
HETATM	6055	OH2	WAT	G	29	72.651	-6.985	94.845	1.00	29.34
HETATM	6056	OH2	WAT	G	30	39.287	9.257	85.623	1.00	22.61
HETATM	6057	OH2	WAT	G	31	61.221	14.462	87.256	1.00	29.85
HETATM	6058	OH2	WAT	G	32	38.167	22.692	107.435	1.00	36.40
HETATM	6059	OH2	WAT	G	33	64.657	-2.682	96.225	1.00	18.70
HETATM	6060	OH2	WAT	G	34	44.059	-2.698	99.805	1.00	30.02
HETATM	6061	OH2	WAT	G	35	38.480	4.763	93.051	1.00	28.03
HETATM	6062	OH2	WAT	G	36	57.899	7.654	112.976	1.00	26.46
HETATM	6063	OH2	WAT	G	37	57.092	3.145	93.309	1.00	22.31
HETATM	6064	OH2	WAT	G	38	52.194	-1.400	118.878	1.00	30.83
HETATM	6065	OH2	WAT	G	39	69.400	14.200	123.379	1.00	30.98
HETATM	6066	OH2	WAT	G	40	24.024	6.540	79.852	1.00	38.13
HETATM	6067	OH2	WAT	G	41	46.657	-10.880	89.402	1.00	29.24
HETATM	6068	OH2	WAT	G	42	24.976	13.489	109.692	1.00	46.34
HETATM	6069	OH2	WAT	G	43	46.533	-4.511	94.759	1.00	23.11
HETATM	6070	OH2	WAT	G	44	51.448	13.833	86.306	1.00	27.08
HETATM	6071	OH2	WAT	G	45	70.578	4.183	105.248	1.00	42.42
HETATM	6072	OH2	WAT	G	46	53.938	-9.936	116.021	1.00	38.97

209/263

Figure 18-93

HETATM 6073	OH2 WAT G	47	38.458	-0.443	63.035	1.00	28.35
HETATM 6074	OH2 WAT G	48	64.786	7.930	107.466	1.00	34.46
HETATM 6075	OH2 WAT G	49	50.823	36.521	114.809	1.00	40.51
HETATM 6076	OH2 WAT G	50	33.963	-10.352	68.080	1.00	39.11
HETATM 6077	OH2 WAT G	51	71.328	-14.321	86.007	1.00	33.30
HETATM 6078	OH2 WAT G	52	63.272	10.210	79.836	1.00	35.75
HETATM 6079	OH2 WAT G	53	59.263	-12.096	94.306	1.00	29.57
HETATM 6080	OH2 WAT G	54	46.041	10.641	76.561	1.00	27.97
HETATM 6081	OH2 WAT G	55	46.614	-13.620	89.775	1.00	24.25
HETATM 6082	OH2 WAT G	56	76.600	0.622	89.097	1.00	29.19
HETATM 6083	OH2 WAT G	57	53.555	6.439	79.089	1.00	34.05
HETATM 6084	OH2 WAT G	58	71.301	11.026	83.310	1.00	35.02
HETATM 6085	OH2 WAT G	59	28.188	-9.956	81.594	1.00	33.21
HETATM 6086	OH2 WAT G	60	53.084	20.992	98.483	1.00	27.64
HETATM 6087	OH2 WAT G	61	59.484	8.630	93.423	1.00	30.30
HETATM 6088	OH2 WAT G	62	26.195	-3.809	95.805	1.00	33.04
HETATM 6089	OH2 WAT G	63	26.095	-0.121	89.620	1.00	37.39
HETATM 6090	OH2 WAT G	64	47.100	-6.141	109.711	1.00	20.88
HETATM 6091	OH2 WAT G	65	23.273	0.731	92.275	1.00	30.38
HETATM 6092	OH2 WAT G	66	45.340	-24.751	72.694	1.00	37.51
HETATM 6093	OH2 WAT G	67	33.754	16.234	111.676	1.00	34.63
HETATM 6094	OH2 WAT G	68	52.831	19.209	126.276	1.00	47.11
HETATM 6095	OH2 WAT G	69	50.218	16.953	111.099	1.00	26.24
HETATM 6096	OH2 WAT G	70	44.791	5.844	70.857	1.00	24.95
HETATM 6097	OH2 WAT G	71	49.517	-18.731	82.921	1.00	29.48
HETATM 6098	OH2 WAT G	72	76.379	10.131	116.550	1.00	48.70
HETATM 6099	OH2 WAT G	73	30.214	-8.086	87.873	1.00	46.35
HETATM 6100	OH2 WAT G	74	45.320	12.061	80.458	1.00	30.80
HETATM 6101	OH2 WAT G	75	72.881	5.360	86.249	1.00	29.04
HETATM 6102	OH2 WAT G	76	59.674	-23.046	87.252	1.00	41.96
HETATM 6103	OH2 WAT G	77	40.619	7.921	100.345	1.00	26.45
HETATM 6104	OH2 WAT G	78	41.666	-19.477	70.073	1.00	36.27
HETATM 6105	OH2 WAT G	79	46.408	-6.539	92.717	1.00	25.78
HETATM 6106	OH2 WAT G	80	35.743	-12.230	81.646	1.00	28.34
HETATM 6107	OH2 WAT G	81	28.268	8.745	121.961	1.00	41.15
HETATM 6108	OH2 WAT G	82	68.843	3.154	71.986	1.00	32.34
HETATM 6109	OH2 WAT G	83	52.125	-11.158	85.150	1.00	24.14
HETATM 6110	OH2 WAT G	84	75.374	-1.773	92.264	1.00	26.12
HETATM 6111	OH2 WAT G	85	46.957	12.230	142.271	1.00	37.07
HETATM 6112	OH2 WAT G	86	63.789	9.551	64.329	1.00	55.58
HETATM 6113	OH2 WAT G	87	60.672	21.185	72.215	1.00	58.55
HETATM 6114	OH2 WAT G	88	56.547	9.505	82.064	1.00	31.10
HETATM 6115	OH2 WAT G	89	26.366	-0.876	92.250	1.00	29.70
HETATM 6116	OH2 WAT G	90	67.604	-16.583	80.808	1.00	32.85
HETATM 6117	OH2 WAT G	91	23.910	1.899	82.068	1.00	42.95
HETATM 6118	OH2 WAT G	92	50.032	4.106	117.380	1.00	30.05
HETATM 6119	OH2 WAT G	93	26.774	-9.492	83.952	1.00	43.59
HETATM 6120	OH2 WAT G	94	42.714	-0.637	113.787	1.00	40.17
HETATM 6121	OH2 WAT G	95	57.966	7.989	134.170	1.00	47.82
HETATM 6122	OH2 WAT G	96	54.478	-3.550	119.086	1.00	36.62
HETATM 6123	OH2 WAT G	97	53.065	11.696	101.718	1.00	41.62
HETATM 6124	OH2 WAT G	98	58.286	-23.645	68.207	1.00	45.98
HETATM 6125	OH2 WAT G	99	54.855	-9.614	121.975	1.00	34.57
HETATM 6126	OH2 WAT G	100	57.408	-3.352	57.145	1.00	42.14
HETATM 6127	OH2 WAT G	101	63.590	20.353	123.667	1.00	33.87
HETATM 6128	OH2 WAT G	102	48.129	-23.143	72.392	1.00	30.23
HETATM 6129	OH2 WAT G	103	62.834	6.913	76.094	1.00	52.01
HETATM 6130	OH2 WAT G	104	34.566	6.529	73.089	1.00	36.29
HETATM 6131	OH2 WAT G	105	51.588	20.869	67.459	1.00	36.85
HETATM 6132	OH2 WAT G	106	28.160	18.020	129.379	1.00	42.87
HETATM 6133	OH2 WAT G	107	49.082	-11.452	57.603	1.00	43.62
HETATM 6134	OH2 WAT G	108	44.717	-8.605	93.281	1.00	41.95
HETATM 6135	OH2 WAT G	109	67.088	-11.900	94.019	1.00	35.71
HETATM 6136	OH2 WAT G	110	49.561	22.763	100.800	1.00	35.40
HETATM 6137	OH2 WAT G	111	75.853	10.960	124.536	1.00	56.20
HETATM 6138	OH2 WAT G	112	54.383	8.930	136.095	1.00	36.40

210/263

Figure 18-94

HETATM 6139	OH2 WAT G 113	33.114	1.764	67.443	1.00	37.01
HETATM 6140	OH2 WAT G 114	42.618	-4.357	102.345	1.00	39.18
HETATM 6141	OH2 WAT G 115	53.605	-10.816	66.281	1.00	31.62
HETATM 6142	OH2 WAT G 116	73.410	-1.010	90.400	1.00	34.72
HETATM 6143	OH2 WAT G 117	68.899	3.789	110.221	1.00	35.69
HETATM 6144	OH2 WAT G 118	31.474	19.159	112.425	1.00	28.08
HETATM 6145	OH2 WAT G 119	39.749	-0.616	132.457	1.00	37.43
HETATM 6146	OH2 WAT G 120	44.921	1.089	137.137	1.00	40.80
HETATM 6147	OH2 WAT G 121	31.081	7.617	75.105	1.00	40.86
HETATM 6148	OH2 WAT G 122	35.554	12.017	105.965	1.00	33.58
HETATM 6149	OH2 WAT G 123	41.381	-23.534	70.872	1.00	38.10
HETATM 6150	OH2 WAT G 124	31.999	1.992	73.813	1.00	33.97
HETATM 6151	OH2 WAT G 125	55.761	10.285	101.654	1.00	47.66
HETATM 6152	OH2 WAT G 126	30.596	12.964	133.642	1.00	37.98
HETATM 6153	OH2 WAT G 127	59.611	5.347	136.114	1.00	46.39
HETATM 6154	OH2 WAT G 128	24.190	12.220	124.679	1.00	30.77
HETATM 6155	OH2 WAT G 129	70.078	4.455	86.283	1.00	36.11
HETATM 6156	OH2 WAT G 130	57.882	-4.314	125.597	1.00	41.40
HETATM 6157	OH2 WAT G 131	45.838	-20.690	65.884	1.00	35.98
HETATM 6158	OH2 WAT G 132	47.574	3.186	79.027	1.00	36.67
HETATM 6159	OH2 WAT G 133	46.856	-18.901	62.295	1.00	45.40
HETATM 6160	OH2 WAT G 134	40.164	5.047	95.358	1.00	31.38
HETATM 6161	OH2 WAT G 135	27.268	-0.405	122.461	1.00	38.16
HETATM 6162	OH2 WAT G 136	54.200	-20.155	66.212	1.00	37.55
HETATM 6163	OH2 WAT G 137	45.435	-10.534	103.626	1.00	37.96
HETATM 6164	OH2 WAT G 138	31.633	25.030	106.499	1.00	43.94
HETATM 6165	OH2 WAT G 139	79.029	-7.518	93.606	1.00	40.55
HETATM 6166	OH2 WAT G 140	68.597	20.711	111.685	1.00	33.25
HETATM 6167	OH2 WAT G 141	64.263	8.524	113.832	1.00	40.63
HETATM 6168	OH2 WAT G 143	49.387	-24.485	70.152	1.00	34.07
HETATM 6169	OH2 WAT G 144	23.383	-3.854	83.604	1.00	32.22
HETATM 6170	OH2 WAT G 145	42.360	-0.710	61.686	1.00	35.94
HETATM 6171	OH2 WAT G 146	34.421	-3.304	65.685	1.00	35.42
HETATM 6172	OH2 WAT G 147	31.506	3.409	89.579	1.00	39.86
HETATM 6173	OH2 WAT G 148	34.963	10.688	91.806	1.00	31.12
HETATM 6174	OH2 WAT G 149	54.859	-15.085	96.769	1.00	46.65
HETATM 6175	OH2 WAT G 150	34.695	2.391	131.273	1.00	39.22
HETATM 6176	OH2 WAT G 151	40.348	1.395	61.905	1.00	34.09
HETATM 6177	OH2 WAT G 152	66.912	17.666	127.489	1.00	45.19
HETATM 6178	OH2 WAT G 153	31.096	19.900	103.232	1.00	43.45
HETATM 6179	OH2 WAT G 154	28.074	-4.222	70.175	1.00	28.86
HETATM 6180	OH2 WAT G 155	63.586	-1.894	99.003	1.00	41.15
HETATM 6181	OH2 WAT G 156	54.145	-22.222	88.415	1.00	40.92
HETATM 6182	OH2 WAT G 157	62.443	13.765	89.547	1.00	33.69
HETATM 6183	OH2 WAT G 158	58.832	9.798	101.311	1.00	31.00
HETATM 6184	OH2 WAT G 159	37.701	-5.528	119.322	1.00	45.00
HETATM 6185	OH2 WAT G 160	43.599	13.442	131.274	1.00	38.43
HETATM 6186	OH2 WAT G 161	23.540	-1.137	96.111	1.00	51.83
HETATM 6187	OH2 WAT G 162	59.915	-4.318	110.873	1.00	41.92
HETATM 6188	OH2 WAT G 163	51.265	-8.264	60.546	1.00	31.25
HETATM 6189	OH2 WAT G 164	58.109	7.024	98.294	1.00	46.30
HETATM 6190	OH2 WAT G 165	46.553	18.195	74.179	1.00	37.53
HETATM 6191	OH2 WAT G 166	55.706	-21.025	92.515	1.00	43.91
HETATM 6192	OH2 WAT G 167	67.146	-1.958	109.704	1.00	43.13
HETATM 6193	OH2 WAT G 168	47.445	-3.047	134.746	1.00	27.99
HETATM 6194	OH2 WAT G 169	65.193	5.304	63.562	1.00	36.05
HETATM 6195	OH2 WAT G 170	36.176	8.979	102.024	1.00	39.63
HETATM 6196	OH2 WAT G 171	70.527	5.797	70.886	1.00	44.69
HETATM 6197	OH2 WAT G 172	67.166	8.735	74.628	1.00	51.41
HETATM 6198	OH2 WAT G 173	19.700	3.630	81.850	1.00	53.49
HETATM 6199	OH2 WAT G 174	55.875	11.277	87.176	1.00	38.63
HETATM 6200	OH2 WAT G 175	61.874	8.432	91.682	1.00	40.08
HETATM 6201	OH2 WAT G 176	36.771	-6.815	121.530	1.00	32.57
HETATM 6202	OH2 WAT G 177	63.224	7.776	89.317	1.00	29.83
HETATM 6203	OH2 WAT G 178	29.606	15.345	132.470	1.00	47.28
HETATM 6204	OH2 WAT G 179	52.811	11.799	98.957	1.00	36.09

211/263

Figure 18-95

HETATM 6205	OH2 WAT G 180	38.589	18.249	88.356	1.00	36.19
HETATM 6206	OH2 WAT G 181	43.734	-15.681	61.135	1.00	34.24
HETATM 6207	OH2 WAT G 182	42.283	15.251	91.437	1.00	37.96
HETATM 6208	OH2 WAT G 183	57.121	-11.129	126.206	1.00	45.78
HETATM 6209	OH2 WAT G 184	50.011	-19.367	92.127	1.00	36.55
HETATM 6210	OH2 WAT G 185	56.880	2.453	95.969	1.00	39.12
HETATM 6211	OH2 WAT G 186	26.356	14.125	125.052	1.00	32.68
HETATM 6212	OH2 WAT G 187	24.631	20.230	122.650	1.00	45.67
HETATM 6213	OH2 WAT G 188	23.516	4.964	81.599	1.00	42.16
HETATM 6214	OH2 WAT G 189	55.017	14.964	62.948	1.00	50.18
HETATM 6215	OH2 WAT G 190	33.371	13.710	105.640	1.00	37.04
HETATM 6216	OH2 WAT G 191	44.466	-10.386	91.144	1.00	36.62
HETATM 6217	OH2 WAT G 192	28.437	22.668	121.285	1.00	38.19
HETATM 6218	OH2 WAT G 193	29.786	24.957	122.112	1.00	42.05
HETATM 6219	OH2 WAT G 194	28.852	3.461	96.101	1.00	48.35
HETATM 6220	OH2 WAT G 195	41.681	11.318	92.011	1.00	32.60
HETATM 6221	OH2 WAT G 196	26.812	-10.229	111.631	1.00	47.70
HETATM 6222	OH2 WAT G 197	42.432	-23.250	76.629	1.00	48.86
HETATM 6223	OH2 WAT G 198	25.484	12.756	121.410	1.00	43.09
HETATM 6224	OH2 WAT G 199	43.514	-20.514	111.706	1.00	46.80
HETATM 6225	OH2 WAT G 200	74.273	-13.079	95.699	1.00	44.89
HETATM 6226	OH2 WAT G 201	59.982	24.381	103.984	1.00	40.63
HETATM 6227	OH2 WAT G 202	67.164	-12.771	74.705	1.00	35.13
HETATM 6228	OH2 WAT G 203	28.708	9.211	79.238	1.00	33.53
HETATM 6229	OH2 WAT G 204	53.256	-3.576	122.243	1.00	48.49
HETATM 6230	OH2 WAT G 205	50.706	16.208	87.357	1.00	41.26
HETATM 6231	OH2 WAT G 206	50.000	34.998	98.339	1.00	39.15
HETATM 6232	OH2 WAT G 207	68.078	-16.236	83.621	1.00	29.70
HETATM 6233	OH2 WAT G 208	24.395	-4.134	111.635	1.00	50.82
HETATM 6234	OH2 WAT G 209	53.384	-2.664	114.289	1.00	44.49
HETATM 6235	OH2 WAT G 210	60.120	-9.482	94.788	1.00	31.97
HETATM 6236	OH2 WAT G 211	23.405	17.472	111.744	1.00	44.97
HETATM 6237	OH2 WAT G 212	46.214	20.943	76.878	1.00	59.14
HETATM 6238	OH2 WAT G 213	29.754	6.983	97.109	1.00	41.78
HETATM 6239	OH2 WAT G 214	46.820	-0.465	55.181	1.00	41.02
HETATM 6240	OH2 WAT G 215	59.143	22.096	124.775	1.00	38.42
HETATM 6241	OH2 WAT G 216	42.674	14.088	66.037	1.00	32.50
HETATM 6242	OH2 WAT G 217	55.009	-7.248	98.186	1.00	56.50
HETATM 6243	OH2 WAT G 218	63.361	-8.209	109.653	1.00	49.66
HETATM 6244	OH2 WAT G 219	66.583	-8.146	94.671	1.00	50.91
HETATM 6245	OH2 WAT G 220	44.627	-2.583	93.919	1.00	36.99
HETATM 6246	OH2 WAT G 221	24.470	-8.606	79.502	1.00	47.24
HETATM 6247	OH2 WAT G 222	76.913	-7.777	83.973	1.00	50.43
HETATM 6248	OH2 WAT G 223	32.788	0.651	129.136	1.00	42.47
HETATM 6249	OH2 WAT G 224	73.731	-16.880	88.817	1.00	46.69
HETATM 6250	OH2 WAT G 225	78.567	-2.802	93.970	1.00	43.17
HETATM 6251	OH2 WAT G 226	45.681	1.248	57.532	1.00	35.84
HETATM 6252	OH2 WAT G 227	38.263	15.236	84.711	1.00	42.39
HETATM 6253	OH2 WAT G 228	38.933	35.224	108.488	1.00	52.23
HETATM 6254	OH2 WAT G 229	33.755	14.939	70.228	1.00	46.56
HETATM 6255	OH2 WAT G 230	51.521	34.184	100.859	1.00	52.96
HETATM 6256	OH2 WAT G 231	34.140	0.565	63.039	1.00	31.02
HETATM 6257	OH2 WAT G 232	37.277	13.977	81.662	1.00	39.83
HETATM 6258	OH2 WAT G 233	57.307	5.947	93.216	1.00	28.55
HETATM 6259	OH2 WAT G 234	31.718	16.820	125.707	1.00	53.16
HETATM 6260	OH2 WAT G 235	60.624	31.119	110.067	1.00	51.02
HETATM 6261	OH2 WAT G 236	44.357	4.267	94.916	1.00	57.50
HETATM 6262	OH2 WAT G 237	68.454	1.072	70.111	1.00	38.65
HETATM 6263	OH2 WAT G 238	27.836	6.773	79.253	1.00	44.95
HETATM 6264	OH2 WAT G 239	54.933	23.344	81.087	1.00	42.95
HETATM 6265	OH2 WAT G 240	34.072	-15.271	71.579	1.00	45.78
HETATM 6266	OH2 WAT G 241	35.966	-1.059	61.973	1.00	38.91
HETATM 6267	OH2 WAT G 242	29.587	1.898	127.376	1.00	44.85
HETATM 6268	OH2 WAT G 243	49.534	-10.150	113.501	1.00	38.32
HETATM 6269	OH2 WAT G 244	57.252	9.773	96.696	1.00	48.83
HETATM 6270	OH2 WAT G 245	62.310	13.262	80.972	1.00	38.54

212/263

Figure 18-96

HETATM 6271	OH2	WAT	G	246	50.248	-5.552	102.815	1.00	43.23
HETATM 6272	OH2	WAT	G	247	47.966	21.564	79.321	1.00	36.79
HETATM 6273	OH2	WAT	G	248	62.507	20.866	108.414	1.00	35.30
HETATM 6274	OH2	WAT	G	249	53.971	19.763	61.067	1.00	47.49
HETATM 6275	OH2	WAT	G	250	38.406	9.828	67.749	1.00	33.71
HETATM 6276	OH2	WAT	G	251	35.304	-6.179	66.319	1.00	36.23
HETATM 6277	OH2	WAT	G	252	39.218	-12.667	85.010	1.00	36.17
HETATM 6278	OH2	WAT	G	253	56.350	5.089	97.225	1.00	46.38
HETATM 6279	OH2	WAT	G	254	69.850	3.406	122.119	1.00	55.07
HETATM 6280	OH2	WAT	G	255	75.703	2.630	128.600	1.00	30.64
HETATM 6281	OH2	WAT	G	256	32.019	-12.973	113.965	1.00	34.48
HETATM 6282	OH2	WAT	G	257	54.081	3.421	56.994	1.00	39.11
HETATM 6283	OH2	WAT	G	258	32.801	-6.170	91.078	1.00	35.72
HETATM 6284	OH2	WAT	G	259	45.040	0.301	95.449	1.00	36.57
HETATM 6285	OH2	WAT	G	260	39.815	21.460	128.855	1.00	40.10
HETATM 6286	OH2	WAT	G	261	28.763	10.408	93.790	1.00	44.39
HETATM 6287	OH2	WAT	G	262	49.668	-12.050	60.539	1.00	50.89
HETATM 6288	OH2	WAT	G	263	64.353	20.015	117.495	1.00	62.67
HETATM 6289	OH2	WAT	G	264	75.183	13.021	128.124	1.00	50.42
HETATM 6290	OH2	WAT	G	265	46.229	6.826	52.485	1.00	46.86
HETATM 6291	OH2	WAT	G	266	68.708	13.973	70.958	1.00	37.90
HETATM 6292	OH2	WAT	G	267	71.504	12.997	130.029	1.00	38.78
HETATM 6293	OH2	WAT	G	268	36.309	-4.716	130.364	1.00	42.92
HETATM 6294	OH2	WAT	G	269	65.973	12.195	79.625	1.00	51.68
HETATM 6295	OH2	WAT	G	270	71.952	13.021	74.292	1.00	37.70
HETATM 6296	OH2	WAT	G	271	44.433	-17.578	62.734	1.00	49.33
HETATM 6297	OH2	WAT	G	272	26.917	15.038	89.067	1.00	38.07
HETATM 6298	OH2	WAT	G	273	63.380	-5.416	126.550	1.00	41.73
HETATM 6299	OH2	WAT	G	274	63.360	-5.356	95.641	1.00	37.54
HETATM 6300	OH2	WAT	G	275	65.947	-13.015	97.485	1.00	37.42
HETATM 6301	OH2	WAT	G	276	26.406	25.831	117.328	1.00	48.37
HETATM 6302	OH2	WAT	G	277	41.893	-10.251	98.201	1.00	46.36
HETATM 6303	OH2	WAT	G	278	30.343	-6.507	117.764	1.00	49.87
HETATM 6304	OH2	WAT	G	279	45.135	32.419	111.056	1.00	43.93
HETATM 6305	OH2	WAT	G	280	50.553	-1.365	120.511	1.00	54.02
HETATM 6306	OH2	WAT	G	281	60.428	13.652	105.130	1.00	31.10
HETATM 6307	OH2	WAT	G	282	30.342	2.204	70.246	1.00	45.19
HETATM 6308	OH2	WAT	G	283	60.358	15.921	127.736	1.00	33.17
HETATM 6309	OH2	WAT	G	284	64.193	3.421	62.117	1.00	45.81
HETATM 6310	OH2	WAT	G	285	45.468	6.113	105.853	1.00	48.98
HETATM 6311	OH2	WAT	G	286	47.514	3.808	98.279	1.00	46.45
HETATM 6312	OH2	WAT	G	287	72.144	-6.345	77.930	1.00	40.04
HETATM 6313	OH2	WAT	G	288	54.142	-5.100	99.674	1.00	43.62
HETATM 6314	OH2	WAT	G	289	48.982	13.297	65.822	1.00	46.98
HETATM 6315	OH2	WAT	G	290	41.171	34.107	115.807	1.00	51.76
HETATM 6316	OH2	WAT	G	291	36.494	37.195	104.170	1.00	44.27
HETATM 6317	OH2	WAT	G	292	48.580	23.117	85.456	1.00	40.96
HETATM 6318	OH2	WAT	G	293	55.853	22.934	98.099	1.00	40.95
HETATM 6319	OH2	WAT	G	294	61.720	11.077	89.427	1.00	41.21
HETATM 6320	OH2	WAT	G	295	43.313	-18.552	114.112	1.00	42.32
HETATM 6321	OH2	WAT	G	296	53.001	-6.305	129.052	1.00	37.41
HETATM 6322	OH2	WAT	G	297	70.258	24.928	82.843	1.00	48.09
HETATM 6323	OH2	WAT	G	298	77.493	0.940	130.507	1.00	51.77
HETATM 6324	OH2	WAT	G	299	32.233	12.182	83.028	1.00	53.51
HETATM 6325	OH2	WAT	G	300	40.666	12.878	65.747	1.00	46.49
HETATM 6326	OH2	WAT	G	301	50.977	12.831	114.597	1.00	48.51
HETATM 6327	OH2	WAT	G	302	54.236	3.817	92.196	1.00	41.15
HETATM 6328	OH2	WAT	G	303	59.527	-1.343	107.471	1.00	36.71
HETATM 6329	OH2	WAT	G	304	70.331	3.940	89.312	1.00	47.70
HETATM 6330	OH2	WAT	G	305	60.626	6.969	127.780	1.00	41.96
HETATM 6331	OH2	WAT	G	306	42.156	-0.139	133.156	1.00	32.19
HETATM 6332	OH2	WAT	G	307	58.886	16.514	99.413	1.00	53.60
HETATM 6333	OH2	WAT	G	308	67.617	-1.589	96.570	1.00	40.36
HETATM 6334	OH2	WAT	G	309	35.868	-10.936	98.849	1.00	48.80
HETATM 6335	OH2	WAT	G	310	45.576	25.388	131.914	1.00	48.99
HETATM 6336	OH2	WAT	G	311	37.583	-6.243	64.257	1.00	37.06

213/263

Figure 18-97

HETATM 6337	OH2 WAT G 312	66.759	16.408	94.600	1.00	45.07
HETATM 6338	OH2 WAT G 313	24.142	11.212	113.340	1.00	52.23
HETATM 6339	OH2 WAT G 314	69.409	16.702	64.230	1.00	39.88
HETATM 6340	OH2 WAT G 315	22.064	24.858	115.328	1.00	50.23
HETATM 6341	OH2 WAT G 316	50.171	9.551	100.345	1.00	37.32
HETATM 6342	OH2 WAT G 317	55.104	31.302	119.497	1.00	44.78
HETATM 6343	OH2 WAT G 318	65.333	-10.105	95.866	1.00	44.21
HETATM 6344	OH2 WAT G 319	31.415	-2.472	128.127	1.00	41.95
HETATM 6345	OH2 WAT G 320	37.423	13.143	88.069	1.00	44.79
HETATM 6346	OH2 WAT G 321	43.619	14.292	96.509	1.00	54.69
HETATM 6347	OH2 WAT G 322	68.048	14.555	126.016	1.00	42.75
HETATM 6348	OH2 WAT G 323	34.778	-2.509	130.204	1.00	37.06
HETATM 6349	OH2 WAT G 324	27.972	18.144	103.841	1.00	47.34
HETATM 6350	OH2 WAT G 325	53.550	23.610	97.592	1.00	38.03
HETATM 6351	OH2 WAT G 326	33.776	4.171	103.451	1.00	50.60
HETATM 6352	OH2 WAT G 327	37.862	35.632	114.870	1.00	48.34
HETATM 6353	OH2 WAT G 328	50.893	14.612	93.478	1.00	38.77
HETATM 6354	OH2 WAT G 329	71.422	-20.913	86.137	1.00	47.69
HETATM 6355	OH2 WAT G 330	50.310	-23.133	74.502	1.00	41.94
HETATM 6356	OH2 WAT G 331	41.520	7.269	60.583	1.00	54.93
HETATM 6357	OH2 WAT G 332	75.879	13.737	106.089	1.00	44.65
HETATM 6358	OH2 WAT G 333	51.923	9.027	138.493	1.00	41.08
HETATM 6359	OH2 WAT G 334	49.511	27.611	79.363	1.00	39.05
HETATM 6360	OH2 WAT G 335	69.385	0.852	110.192	1.00	41.42
HETATM 6361	OH2 WAT G 336	40.952	2.479	101.880	1.00	42.50
HETATM 6362	OH2 WAT G 337	32.998	7.200	103.784	1.00	54.22
HETATM 6363	OH2 WAT G 338	54.366	15.261	136.205	1.00	52.69
HETATM 6364	OH2 WAT G 339	35.674	13.727	89.792	1.00	35.83
HETATM 6365	OH2 WAT G 340	66.606	-21.361	87.138	1.00	46.26
HETATM 6366	OH2 WAT G 341	72.053	4.708	131.550	1.00	45.27
HETATM 6367	OH2 WAT G 342	28.072	-1.358	70.419	1.00	34.92
HETATM 6368	OH2 WAT G 343	23.611	-3.981	76.422	1.00	52.99
HETATM 6369	OH2 WAT G 344	53.684	2.564	122.150	1.00	58.16
HETATM 6370	OH2 WAT G 345	30.624	-6.528	125.556	1.00	34.71
HETATM 6371	OH2 WAT G 346	27.870	13.838	113.997	1.00	44.91
HETATM 6372	OH2 WAT G 347	31.903	-9.588	116.327	1.00	55.34
HETATM 6373	OH2 WAT G 348	71.763	15.094	63.739	1.00	48.99
HETATM 6374	OH2 WAT G 349	25.258	-2.536	114.760	1.00	37.19
HETATM 6375	OH2 WAT G 350	43.765	12.162	78.143	1.00	42.32
HETATM 6376	OH2 WAT G 351	32.452	5.338	73.909	1.00	33.70
HETATM 6377	OH2 WAT G 352	52.896	-5.770	101.894	1.00	46.40
HETATM 6378	OH2 WAT G 353	47.968	4.242	115.852	1.00	34.62
HETATM 6379	OH2 WAT G 354	38.561	-9.302	90.596	1.00	49.80
HETATM 6380	OH2 WAT G 355	63.791	17.454	74.354	1.00	56.40
HETATM 6381	OH2 WAT G 356	41.360	2.648	133.760	1.00	50.00
HETATM 6382	OH2 WAT G 357	42.467	-7.937	122.328	1.00	38.01
HETATM 6383	OH2 WAT G 358	50.890	-0.362	116.668	1.00	39.26
HETATM 6384	OH2 WAT G 359	54.217	-23.881	67.865	1.00	55.18
HETATM 6385	OH2 WAT G 360	64.959	9.539	105.032	1.00	38.83
HETATM 6386	OH2 WAT G 361	58.113	-19.846	82.288	1.00	38.60
HETATM 6387	OH2 WAT G 362	42.245	-1.140	93.572	1.00	31.47
HETATM 6388	OH2 WAT G 363	73.552	17.770	125.885	1.00	54.89
HETATM 6389	OH2 WAT G 364	68.769	15.898	106.810	1.00	45.53
HETATM 6390	OH2 WAT G 365	37.543	19.031	78.866	1.00	45.15
HETATM 6391	OH2 WAT G 366	55.583	6.906	95.087	1.00	44.99
HETATM 6392	OH2 WAT G 367	41.284	9.699	78.250	1.00	36.58
HETATM 6393	OH2 WAT G 368	25.203	5.332	126.362	1.00	46.60
HETATM 6394	OH2 WAT G 369	74.742	-5.006	95.104	1.00	47.85
HETATM 6395	OH2 WAT G 370	70.349	19.871	69.925	1.00	51.46
HETATM 6396	OH2 WAT G 371	42.936	20.631	94.720	1.00	38.66
HETATM 6397	OH2 WAT G 372	34.162	-16.114	114.141	1.00	44.01
HETATM 6398	OH2 WAT G 373	33.863	16.838	100.275	1.00	44.66
HETATM 6399	OH2 WAT G 374	21.613	12.569	86.140	1.00	43.89
HETATM 6400	OH2 WAT G 375	35.751	-13.302	100.583	1.00	53.53
HETATM 6401	OH2 WAT G 376	70.095	13.395	117.505	1.00	52.02
HETATM 6402	OH2 WAT G 377	41.853	19.108	131.799	1.00	46.47

214/263

Figure 18-98

HETATM 6403	OH2	WAT	G	378	55.780	-14.986	65.487	1.00	49.09
HETATM 6404	OH2	WAT	G	379	40.990	21.205	91.611	1.00	41.02
HETATM 6405	OH2	WAT	G	380	48.157	1.057	116.992	1.00	44.84
HETATM 6406	OH2	WAT	G	381	37.954	-6.221	128.334	1.00	37.09
HETATM 6407	OH2	WAT	G	382	30.221	27.743	109.194	1.00	39.92
HETATM 6408	OH2	WAT	G	383	49.926	-12.826	118.421	1.00	58.95
HETATM 6409	OH2	WAT	G	384	42.435	-17.636	81.477	1.00	48.47
HETATM 6410	OH2	WAT	G	385	58.226	-25.990	71.378	1.00	48.18
HETATM 6411	OH2	WAT	G	386	40.495	17.944	128.741	1.00	43.82
HETATM 6412	OH2	WAT	G	387	31.943	6.301	109.475	1.00	35.53
HETATM 6413	OH2	WAT	G	388	47.277	2.559	100.509	1.00	43.00
HETATM 6414	OH2	WAT	G	389	38.862	9.112	102.620	1.00	31.70
HETATM 6415	OH2	WAT	G	390	71.652	14.568	105.167	1.00	49.63
HETATM 6416	OH2	WAT	G	391	68.554	-10.518	73.331	1.00	38.16
HETATM 6417	OH2	WAT	G	392	70.496	-16.160	84.425	1.00	32.16
HETATM 6418	OH2	WAT	G	393	44.698	-24.950	75.603	1.00	43.38
HETATM 6419	OH2	WAT	G	394	56.172	15.369	55.027	1.00	47.44
HETATM 6420	OH2	WAT	G	395	46.150	-9.441	99.999	1.00	47.98
HETATM 6421	OH2	WAT	G	396	26.892	-8.356	89.057	1.00	34.99
HETATM 6422	OH2	WAT	G	397	31.737	14.380	90.395	1.00	50.78
HETATM 6423	OH2	WAT	G	398	36.261	-13.824	62.777	1.00	50.86
HETATM 6424	OH2	WAT	G	399	37.312	15.242	134.977	1.00	43.57
HETATM 6425	OH2	WAT	G	400	33.728	13.773	126.419	1.00	57.13
HETATM 6426	OH2	WAT	G	401	45.269	27.937	130.311	1.00	49.55
HETATM 6427	OH2	WAT	G	402	44.887	-17.414	111.508	1.00	54.29
HETATM 6428	OH2	WAT	G	403	68.928	0.455	136.711	1.00	49.90
HETATM 6429	OH2	WAT	G	404	43.271	-21.571	64.425	1.00	48.61
HETATM 6430	OH2	WAT	G	405	24.243	-4.781	108.590	1.00	51.05
HETATM 6431	OH2	WAT	G	406	54.828	5.311	59.009	1.00	43.43
HETATM 6432	OH2	WAT	G	407	53.460	27.992	124.076	1.00	47.83
HETATM 6433	OH2	WAT	G	408	70.833	-18.390	85.386	1.00	49.26
HETATM 6434	OH2	WAT	G	409	71.497	15.287	113.071	1.00	34.52
HETATM 6435	OH2	WAT	G	410	36.407	-18.480	110.466	1.00	55.43
HETATM 6436	OH2	WAT	G	411	26.220	-9.551	78.158	1.00	47.69
HETATM 6437	OH2	WAT	G	412	52.319	26.326	82.038	1.00	42.00
HETATM 6438	OH2	WAT	G	413	76.173	14.097	122.253	1.00	44.90
HETATM 6439	OH2	WAT	G	414	58.379	6.335	123.024	1.00	54.61
HETATM 6440	OH2	WAT	G	415	72.162	-16.705	82.719	1.00	50.63
HETATM 6441	OH2	WAT	G	416	63.557	26.152	65.944	1.00	39.83
HETATM 6442	OH2	WAT	G	417	38.935	23.070	122.742	1.00	52.57
HETATM 6443	OH2	WAT	G	418	55.256	-10.714	124.501	1.00	42.38
HETATM 6444	OH2	WAT	G	419	55.443	-9.037	110.170	1.00	46.47
HETATM 6445	OH2	WAT	G	420	73.873	16.578	123.288	1.00	46.54
HETATM 6446	OH2	WAT	G	421	74.426	12.663	117.527	1.00	43.62
HETATM 6447	OH2	WAT	G	422	52.374	-0.368	51.502	1.00	56.99
HETATM 6448	OH2	WAT	G	423	60.339	20.215	84.713	1.00	36.27
HETATM 6449	OH2	WAT	G	424	48.308	1.354	54.561	1.00	38.53
HETATM 6450	OH2	WAT	G	425	61.757	21.606	115.976	1.00	61.09
HETATM 6451	OH2	WAT	G	426	33.222	-14.916	119.528	1.00	51.12
HETATM 6452	OH2	WAT	G	427	47.477	3.359	112.298	1.00	46.10
HETATM 6453	OH2	WAT	G	428	39.909	2.272	138.388	1.00	35.33
HETATM 6454	OH2	WAT	G	429	57.829	15.336	126.262	1.00	62.59
HETATM 6455	OH2	WAT	G	430	48.917	-5.857	119.191	1.00	51.45
HETATM 6456	OH2	WAT	G	431	44.139	-3.812	132.964	1.00	44.91
HETATM 6457	OH2	WAT	G	432	38.885	18.594	95.398	1.00	50.23
HETATM 6458	OH2	WAT	G	433	52.628	-7.064	55.271	1.00	38.96
HETATM 6459	OH2	WAT	G	434	60.644	-0.731	101.129	1.00	47.30
HETATM 6460	OH2	WAT	G	435	64.772	5.808	71.942	1.00	50.81
HETATM 6461	OH2	WAT	G	436	39.571	16.705	80.180	1.00	34.07
HETATM 6462	OH2	WAT	G	437	32.791	-0.551	65.371	1.00	41.40
HETATM 6463	OH2	WAT	G	438	58.318	-7.989	60.087	1.00	46.94
HETATM 6464	OH2	WAT	G	439	26.982	5.474	120.408	1.00	46.28
HETATM 6465	OH2	WAT	G	440	72.138	1.233	90.050	1.00	50.13
HETATM 6466	OH2	WAT	G	441	29.494	10.971	118.393	1.00	56.30
HETATM 6467	OH2	WAT	G	442	69.232	5.594	113.941	1.00	58.17
HETATM 6468	OH2	WAT	G	443	61.459	11.576	71.140	1.00	61.67

215/263
Figure 18-99

HETATM 6469	OH2 WAT G 444	59.592	2.195	58.518	1.00	42.66
HETATM 6470	OH2 WAT G 445	47.407	6.152	111.310	1.00	45.14
HETATM 6471	OH2 WAT G 446	36.254	18.203	99.930	1.00	44.76
HETATM 6472	OH2 WAT G 447	49.525	32.050	116.235	1.00	47.72
HETATM 6473	OH2 WAT G 448	21.801	-5.358	81.109	1.00	42.07
HETATM 6474	OH2 WAT G 449	52.131	-14.007	95.380	1.00	40.76
HETATM 6475	OH2 WAT G 450	39.712	-19.983	72.499	1.00	51.69
HETATM 6476	OH2 WAT G 451	67.651	5.620	67.102	1.00	42.38
HETATM 6477	OH2 WAT G 452	77.344	1.313	79.207	1.00	63.64
HETATM 6478	OH2 WAT G 453	55.249	-29.426	86.187	1.00	44.98
HETATM 6479	OH2 WAT G 454	64.429	-11.004	98.104	1.00	49.12
HETATM 6480	OH2 WAT G 455	45.456	-0.814	129.510	1.00	61.60
HETATM 6481	OH2 WAT G 456	65.066	-14.790	68.028	1.00	40.08
HETATM 6482	OH2 WAT G 457	34.732	5.611	94.924	1.00	58.32

216/263

Figure 19-1

				Residue #	X	Y	Z	B	Segment	ID
ATOM	1	CB	ALA	2	45.368	37.329	75.022	1.00	57.10	AAAA
ATOM	2	C	ALA	2	46.761	38.761	73.244	1.00	55.49	AAAA
ATOM	3	O	ALA	2	46.339	39.800	73.750	1.00	55.57	AAAA
ATOM	4	N	ALA	2	48.280	37.746	74.937	1.00	57.26	AAAA
ATOM	5	CA	ALA	2	47.062	37.537	74.110	1.00	56.37	AAAA
ATOM	6	H	LYS	3	46.976	38.628	71.938	1.00	53.94	AAAA
ATOM	7	CA	LYS	3	46.721	39.716	71.002	1.00	51.97	AAAA
ATOM	8	CE	LYS	3	47.815	39.778	69.939	1.00	53.86	AAAA
ATOM	9	CG	LYS	3	49.223	39.876	70.490	1.00	56.47	AAAA
ATOM	10	CD	LYS	3	50.252	39.670	69.387	1.00	57.84	AAAA
ATOM	11	CE	LYS	3	51.654	39.597	69.957	1.00	58.89	AAAA
ATOM	12	NZ	LYS	3	52.643	39.283	68.895	1.00	59.33	AAAA
ATOM	13	C	LYS	3	45.393	39.494	70.305	1.00	49.57	AAAA
ATOM	14	O	LYS	3	44.894	38.373	70.246	1.00	49.33	AAAA
ATOM	15	N	VAL	4	44.826	40.574	69.777	1.00	46.23	AAAA
ATOM	16	CA	VAL	4	43.561	40.516	69.056	1.00	42.51	AAAA
ATOM	17	CB	VAL	4	42.543	41.516	69.630	1.00	42.26	AAAA
ATOM	18	CG1	VAL	4	41.213	41.352	68.940	1.00	41.51	AAAA
ATOM	19	CG2	VAL	4	42.401	41.307	71.128	1.00	42.00	AAAA
ATOM	20	C	VAL	4	43.918	40.913	67.638	1.00	39.94	AAAA
ATOM	21	O	VAL	4	44.332	42.032	67.395	1.00	40.39	AAAA
ATOM	22	N	LYS	5	43.766	40.001	56.695	1.00	36.94	AAAA
ATOM	23	CA	LYS	5	44.142	40.305	65.323	1.00	34.10	AAAA
ATOM	24	CB	LYS	5	45.179	39.290	64.846	1.00	35.02	AAAA
ATOM	25	CG	LYS	5	46.424	39.182	65.698	1.00	34.07	AAAA
ATOM	26	CD	LYS	5	47.233	40.452	65.652	1.00	33.44	AAAA
ATOM	27	CE	LYS	5	48.565	40.239	66.333	1.00	32.38	AAAA
ATOM	28	NZ	LYS	5	49.372	41.460	66.222	1.00	31.26	AAAA
ATOM	29	C	LYS	5	42.997	40.293	64.333	1.00	31.38	AAAA
ATOM	30	O	LYS	5	42.053	39.523	64.466	1.00	31.74	AAAA
ATOM	31	N	LEU	6	43.090	41.142	63.326	1.00	28.60	AAAA
ATOM	32	CA	LEU	6	42.075	41.167	62.289	1.00	26.90	AAAA
ATOM	33	CB	LEU	6	41.530	42.580	62.067	1.00	26.43	AAAA
ATOM	34	CS	LEU	6	40.321	42.748	61.129	1.00	25.89	AAAA
ATOM	35	CD1	LEU	6	40.108	44.224	60.826	1.00	25.50	AAAA
ATOM	36	CD2	LEU	6	40.550	42.032	59.828	1.00	26.64	AAAA
ATOM	37	C	LEU	6	42.818	40.701	61.049	1.00	25.74	AAAA
ATOM	38	O	LEU	6	43.877	41.226	60.717	1.00	24.60	AAAA
ATOM	39	H	LEU	6	42.282	39.704	60.367	1.00	25.90	AAAA
ATOM	40	CA	LEU	7	42.939	39.212	59.173	1.00	26.75	AAAA
ATOM	41	CB	LEU	7	42.839	37.712	59.089	1.00	26.58	AAAA
ATOM	42	CG2	LEU	7	43.474	37.227	57.783	1.00	27.88	AAAA
ATOM	43	CG1	LEU	7	43.528	37.116	60.310	1.00	27.02	AAAA
ATOM	44	CD1	LEU	7	43.507	35.640	60.350	1.00	27.46	AAAA
ATOM	45	C	LEU	7	42.339	39.814	57.929	1.00	26.70	AAAA
ATOM	46	O	LEU	7	41.162	39.655	57.681	1.00	27.68	AAAA
ATOM	47	N	GLY	8	43.144	40.509	57.142	1.00	27.94	AA A
ATOM	48	CA	GLY	8	42.598	41.110	55.944	1.00	29.78	AA A
ATOM	49	C	GLY	8	43.587	41.739	55.027	1.00	30.38	AAAA
ATOM	50	O	GLY	8	44.785	41.765	55.264	1.00	29.39	AAAA
ATOM	51	N	THR	9	43.051	42.395	53.971	1.00	31.84	AAAA
ATOM	52	CA	THR	9	43.832	43.106	52.962	1.00	32.41	AAAA
ATOM	53	CB	THR	9	44.606	42.112	52.064	1.00	31.12	AAAA
ATOM	54	CG1	THR	9	45.324	42.825	51.053	1.00	30.74	AAAA
ATOM	55	CG2	THR	9	43.654	41.140	51.411	1.00	30.27	AAAA
ATOM	56	C	THR	9	42.886	43.939	52.091	1.00	32.94	AAAA
ATOM	57	O	THR	9	41.705	43.625	51.993	1.00	33.62	AAAA
ATOM	58	N	LEU	10	43.396	45.009	51.485	1.00	33.20	AAAA
ATOM	59	CA	LEU	10	42.573	45.840	50.611	1.00	33.29	AAAA
ATOM	60	CB	LEU	10	43.117	47.275	50.484	1.00	33.12	AAAA
ATOM	61	CG	LEU	10	43.142	48.245	51.566	1.00	32.95	AAAA
ATOM	62	CD1	LEU	10	41.743	48.336	52.288	1.00	31.99	AAAA
ATOM	63	CD2	LEU	10	44.126	47.734	52.575	1.00	34.71	AAAA
ATOM	64	C	LEU	10	42.527	45.231	49.218	1.00	33.18	AAAA
ATOM	65	O	LEU	10	41.876	45.758	48.328	1.00	32.52	AAAA
ATOM	66	H	ASP	11	43.230	44.121	49.022	1.00	33.56	AAAA

217/263

Figure 19-2

ATOM	67	CA	ASP	A	11	43.240	43.489	47.716	1.00	34.24	AAAA
ATOM	68	CB	ASP	A	11	44.393	42.499	47.607	1.00	35.81	AAAA
ATOM	69	CG	ASP	A	11	45.739	43.190	47.604	1.00	37.57	AAAA
ATOM	70	OD1	ASP	A	11	45.890	44.178	46.855	1.00	37.95	AAAA
ATOM	71	OD2	ASP	A	11	46.650	42.750	48.332	1.00	40.31	AAAA
ATOM	72	C	ASP	A	11	41.929	42.813	47.341	1.00	34.03	AAAA
ATOM	73	O	ASP	A	11	41.629	42.652	46.150	1.00	34.80	AAAA
ATOM	74	N	TYR	A	12	41.142	42.417	48.335	1.00	32.34	AAAA
ATOM	75	CA	TYR	A	12	39.871	41.803	48.017	1.00	32.53	AAAA
ATOM	76	CB	TYR	A	12	39.043	41.569	49.290	1.00	31.32	AAAA
ATOM	77	CG	TYR	A	12	39.551	40.438	50.162	1.00	29.95	AAAA
ATOM	78	CD1	TYR	A	12	39.983	40.669	51.469	1.00	28.52	AAAA
ATOM	79	CE1	TYR	A	12	40.413	39.614	52.279	1.00	28.03	AAAA
ATOM	80	CD2	TYR	A	12	39.568	39.128	49.688	1.00	28.47	AAAA
ATOM	81	CE2	TYR	A	12	39.992	38.083	50.483	1.00	28.47	AAAA
ATOM	82	CZ	TYR	A	12	40.408	38.330	51.775	1.00	28.43	AAAA
ATOM	83	OH	TYR	A	12	40.786	37.277	52.569	1.00	29.86	AAAA
ATOM	84	C	TYR	A	12	39.146	42.749	47.066	1.00	33.16	AAAA
ATOM	85	O	TYR	A	12	38.554	42.324	46.082	1.00	33.36	AAAA
ATOM	86	N	GLY	A	13	39.237	44.041	47.356	1.00	34.76	AAAA
ATOM	87	CA	GLY	A	13	38.594	45.065	46.546	1.00	36.60	AAAA
ATOM	88	C	GLY	A	13	38.814	44.961	45.052	1.00	37.85	AAAA
ATOM	89	O	GLY	A	13	38.105	45.591	44.275	1.00	37.40	AAAA
ATOM	90	N	LYS	A	14	39.799	44.171	44.647	1.00	39.55	AAAA
ATOM	91	CA	LYS	A	14	40.091	43.981	43.231	1.00	40.66	AAAA
ATOM	92	CB	LYS	A	14	41.605	43.977	42.995	1.00	42.26	AAAA
ATOM	93	CG	LYS	A	14	42.300	45.309	43.239	1.00	44.54	AAAA
ATOM	94	CD	LYS	A	14	41.820	46.445	42.304	1.00	46.32	AAAA
ATOM	95	CE	LYS	A	14	42.033	46.158	40.810	1.00	46.64	AAAA
ATOM	96	NZ	LYS	A	14	41.133	45.086	40.256	1.00	47.23	AAAA
ATOM	97	C	LYS	A	14	39.499	42.675	42.707	1.00	40.35	AAAA
ATOM	98	O	LYS	A	14	39.593	42.377	41.511	1.00	39.97	AAAA
ATOM	99	N	TYR	A	15	38.897	41.901	43.605	1.00	39.95	AAAA
ATOM	100	CA	TYR	A	15	38.300	40.617	43.245	1.00	40.30	AAAA
ATOM	101	CB	TYR	A	15	38.962	39.490	44.050	1.00	38.46	AAAA
ATOM	102	CG	TYR	A	15	40.472	39.519	44.021	1.00	37.01	AAAA
ATOM	103	CD1	TYR	A	15	41.213	39.136	45.137	1.00	36.24	AAAA
ATOM	104	CE1	TYR	A	15	42.604	39.220	45.144	1.00	35.73	AAAA
ATOM	105	CD2	TYR	A	15	41.163	39.976	42.902	1.00	36.84	AAAA
ATOM	106	CE2	TYR	A	15	42.556	40.064	42.898	1.00	36.53	AAAA
ATOM	107	CZ	TYR	A	15	43.271	39.689	44.028	1.00	36.24	AAAA
ATOM	108	OH	TYR	A	15	44.648	39.816	44.042	1.00	36.49	AAAA
ATOM	109	C	TYR	A	15	36.802	40.647	43.556	1.00	41.98	AAAA
ATOM	110	O	TYR	A	15	36.288	39.786	44.280	1.00	42.59	AAAA
ATOM	111	N	ARG	A	16	36.101	41.638	43.014	1.00	42.81	AAAA
ATOM	112	CA	ARG	A	16	34.670	41.753	43.257	1.00	43.47	AAAA
ATOM	113	CB	ARG	A	16	34.205	43.197	43.111	1.00	45.27	AAAA
ATOM	114	CG	ARG	A	16	35.021	44.234	43.833	1.00	48.06	AAAA
ATOM	115	CD	ARG	A	16	34.891	44.196	45.339	1.00	49.63	AAAA
ATOM	116	NE	ARG	A	16	35.632	45.322	45.905	1.00	51.65	AAAA
ATOM	117	CZ	ARG	A	16	35.382	46.602	45.622	1.00	52.71	AAAA
ATOM	118	NH1	ARG	A	16	34.406	46.931	44.781	1.00	53.28	AAAA
ATOM	119	NH2	ARG	A	16	36.124	47.560	46.162	1.00	53.43	AAAA
ATOM	120	C	ARG	A	16	33.913	40.929	42.230	1.00	42.86	AAAA
ATOM	121	O	ARG	A	16	34.455	40.541	41.193	1.00	41.83	AAAA
ATOM	122	N	TYR	A	17	32.651	40.668	42.523	1.00	42.42	AAAA
ATOM	123	CA	TYR	A	17	31.818	39.942	41.590	1.00	42.76	AAAA
ATOM	124	CB	TYR	A	17	30.675	39.254	42.333	1.00	40.11	AAAA
ATOM	125	CG	TYR	A	17	31.097	38.061	43.180	1.00	38.35	AAAA
ATOM	126	CD1	TYR	A	17	32.169	38.148	44.071	1.00	36.15	AAAA
ATOM	127	CE1	TYR	A	17	32.519	37.069	44.874	1.00	34.76	AAAA
ATOM	128	CD2	TYR	A	17	30.386	36.855	43.116	1.00	36.40	AAAA
ATOM	129	CE2	TYR	A	17	30.726	35.776	43.912	1.00	35.31	AAAA
ATOM	130	CZ	TYR	A	17	31.792	35.887	44.790	1.00	35.00	AAAA
ATOM	131	OH	TYR	A	17	32.115	34.814	45.584	1.00	33.29	AAAA
ATOM	132	C	TYR	A	17	31.296	41.000	40.613	1.00	44.43	AAAA

218/263 Figure 19-3

ATOM	133	O	TYR	A	17	31.346	42.194	40.905	1.00	44.68	AAAA
ATOM	134	N	PRO	A	18	30.799	40.574	39.440	1.00	45.95	AAAA
ATOM	135	CD	PRO	A	18	30.707	39.175	38.994	1.00	46.08	AAAA
ATOM	136	CA	PRO	A	18	30.268	41.465	38.402	1.00	47.24	AAAA
ATOM	137	CB	PRO	A	18	29.854	40.482	37.312	1.00	47.69	AAAA
ATOM	138	CG	PRO	A	18	30.876	39.338	37.511	1.00	46.79	AAAA
ATOM	139	C	PRO	A	18	29.129	42.390	38.834	1.00	48.98	AAAA
ATOM	140	O	PRO	A	18	28.298	42.020	39.660	1.00	49.11	AAAA
ATOM	141	N	LYS	A	19	29.114	43.593	38.253	1.00	50.59	AAAA
ATOM	142	CA	LYS	A	19	28.125	44.654	38.519	1.00	52.10	AAAA
ATOM	143	CB	LYS	A	19	27.876	45.466	37.246	1.00	54.41	AAAA
ATOM	144	CG	LYS	A	19	29.120	45.911	36.498	1.00	57.78	AAAA
ATOM	145	CD	LYS	A	19	28.747	46.508	35.142	1.00	59.34	AAAA
ATOM	146	CE	LYS	A	19	29.978	46.774	34.288	1.00	60.33	AAAA
ATOM	147	NZ	LYS	A	19	29.616	47.277	32.932	1.00	61.03	AAAA
ATOM	148	C	LYS	A	19	26.764	44.162	39.012	1.00	51.53	AAAA
ATOM	149	O	LYS	A	19	26.281	44.556	40.071	1.00	51.54	AAAA
ATOM	150	N	ASN	A	20	26.146	43.314	38.203	1.00	50.13	AAAA
ATOM	151	CA	ASN	A	20	24.831	42.750	38.482	1.00	48.44	AAAA
ATOM	152	CB	ASN	A	20	24.336	42.061	37.209	1.00	49.67	AAAA
ATOM	153	CG	ASN	A	20	25.389	41.132	36.613	1.00	51.61	AAAA
ATOM	154	OD1	ASN	A	20	25.677	40.064	37.154	1.00	51.70	AAAA
ATOM	155	ND2	ASN	A	20	25.998	41.562	35.509	1.00	53.00	AAAA
ATOM	156	C	ASN	A	20	24.789	41.765	39.649	1.00	45.57	AAAA
ATOM	157	O	ASN	A	20	23.764	41.127	39.877	1.00	44.67	AAAA
ATOM	158	N	HIS	A	21	25.883	41.662	40.398	1.00	42.71	AAAA
ATOM	159	CA	HIS	A	21	25.958	40.709	41.506	1.00	40.69	AAAA
ATOM	160	CB	HIS	A	21	27.216	39.857	41.353	1.00	40.16	AAAA
ATOM	161	CG	HIS	A	21	27.186	38.587	42.140	1.00	39.93	AAAA
ATOM	162	CD2	HIS	A	21	27.329	38.353	43.467	1.00	39.27	AAAA
ATOM	163	ND1	HIS	A	21	26.951	37.359	41.557	1.00	39.47	AAAA
ATOM	164	CE1	HIS	A	21	26.948	36.425	42.493	1.00	39.36	AAAA
ATOM	165	NE2	HIS	A	21	27.174	37.003	43.660	1.00	39.44	AAAA
ATOM	166	C	HIS	A	21	25.974	41.349	42.892	1.00	38.93	AAAA
ATOM	167	O	HIS	A	21	26.660	42.338	43.116	1.00	38.78	AAAA
ATOM	168	N	PRO	A	22	25.229	40.778	43.853	1.00	37.11	AAAA
ATOM	169	CD	PRO	A	22	24.371	39.579	43.814	1.00	36.09	AAAA
ATOM	170	CA	PRO	A	22	25.224	41.361	45.199	1.00	35.81	AAAA
ATOM	171	CB	PRO	A	22	24.473	40.306	46.012	1.00	36.04	AAAA
ATOM	172	CG	PRO	A	22	23.464	39.810	45.003	1.00	36.19	AAAA
ATOM	173	C	PRO	A	22	26.638	41.637	45.751	1.00	34.39	AAAA
ATOM	174	O	PRO	A	22	26.867	42.653	46.417	1.00	34.09	AAAA
ATOM	175	N	LEU	A	23	27.572	40.731	45.451	1.00	31.98	AAAA
ATOM	176	CA	LEU	A	23	28.954	40.827	45.900	1.00	29.65	AAAA
ATOM	177	CB	LEU	A	23	29.564	39.432	46.014	1.00	27.88	AAAA
ATOM	178	CG	LEU	A	23	28.896	38.528	47.048	1.00	27.31	AAAA
ATOM	179	CD1	LEU	A	23	29.656	37.217	47.149	1.00	26.64	AAAA
ATOM	180	CD2	LEU	A	23	28.879	39.212	48.399	1.00	26.75	AAAA
ATOM	181	C	LEU	A	23	29.838	41.709	45.018	1.00	29.20	AAAA
ATOM	182	O	LEU	A	23	31.057	41.606	45.028	1.00	28.38	AAAA
ATOM	183	N	LYS	A	24	29.204	42.582	44.259	1.00	29.27	AAAA
ATOM	184	CA	LYS	A	24	29.903	43.512	43.389	1.00	29.30	AAAA
ATOM	185	CB	LYS	A	24	28.881	44.091	42.405	1.00	29.75	AAAA
ATOM	186	CG	LYS	A	24	29.328	45.265	41.601	1.00	32.55	AAAA
ATOM	187	CD	LYS	A	24	28.537	46.526	41.994	1.00	34.37	AAAA
ATOM	188	CE	LYS	A	24	27.025	46.337	41.835	1.00	34.32	AAAA
ATOM	189	NZ	LYS	A	24	26.221	47.542	42.208	1.00	34.37	AAAA
ATOM	190	C	LYS	A	24	30.580	44.620	44.224	1.00	28.14	AAAA
ATOM	191	O	LYS	A	24	31.617	45.162	43.840	1.00	27.93	AAAA
ATOM	192	N	ILE	A	25	29.990	44.919	45.377	1.00	27.07	AAAA
ATOM	193	CA	ILE	A	25	30.468	45.945	46.296	1.00	25.82	AAAA
ATOM	194	CB	ILE	A	25	29.425	46.262	47.364	1.00	25.37	AAAA
ATOM	195	CG2	ILE	A	25	28.190	46.846	46.737	1.00	25.71	AAAA
ATOM	196	CG1	ILE	A	25	29.142	44.979	48.157	1.00	25.26	AAAA
ATOM	197	CD1	ILE	A	25	28.318	45.163	49.413	1.00	25.17	AAAA
ATOM	198	C	ILE	A	25	31.700	45.550	47.095	1.00	25.28	AAAA

219/263

Figure 19-4

ATOM	199	O	ILE	A	25	32.037	44.379	47.183	1.00	24.48	AAAA
ATOM	200	N	PRO	A	26	32.375	46.547	47.714	1.00	24.98	AAAA
ATOM	201	CD	PRO	A	26	32.062	47.980	47.638	1.00	24.98	AAAA
ATOM	202	CA	PRO	A	26	33.570	46.367	48.543	1.00	24.44	AAAA
ATOM	203	CB	PRO	A	26	34.094	47.792	48.701	1.00	24.75	AAAA
ATOM	204	CG	PRO	A	26	33.435	48.546	47.538	1.00	25.51	AAAA
ATOM	205	C	PRO	A	26	33.021	45.838	49.862	1.00	23.42	AAAA
ATOM	206	O	PRO	A	26	31.930	46.233	50.272	1.00	22.12	AAAA
ATOM	207	N	ARG	A	27	33.754	44.960	50.532	1.00	23.06	AAAA
ATOM	208	CA	ARG	A	27	33.244	44.421	51.776	1.00	23.04	AAAA
ATOM	209	CB	ARG	A	27	32.633	43.043	51.492	1.00	22.20	AAAA
ATOM	210	CG	ARG	A	27	31.463	43.152	50.503	1.00	19.84	AAAA
ATOM	211	CD	ARG	A	27	30.762	41.844	50.160	1.00	18.64	AAAA
ATOM	212	NE	ARG	A	27	30.181	41.168	51.315	1.00	16.51	AAAA
ATOM	213	CZ	ARG	A	27	30.774	40.188	51.982	1.00	16.57	AAAA
ATOM	214	NH1	ARG	A	27	31.969	39.763	51.605	1.00	17.50	AAAA
ATOM	215	NH2	ARG	A	27	30.185	39.643	53.038	1.00	16.45	AAAA
ATOM	216	C	ARG	A	27	34.265	44.381	52.905	1.00	23.62	AAAA
ATOM	217	O	ARG	A	27	34.107	45.077	53.919	1.00	23.69	AAAA
ATOM	218	N	VAL	A	28	35.305	43.570	52.736	1.00	24.25	AAAA
ATOM	219	CA	VAL	A	28	36.355	43.466	53.737	1.00	23.36	AAAA
ATOM	220	CB	VAL	A	28	37.022	42.062	53.671	1.00	22.75	AAAA
ATOM	221	CG1	VAL	A	28	38.292	42.031	54.475	1.00	22.95	AAAA
ATOM	222	CG2	VAL	A	28	36.061	41.011	54.249	1.00	22.20	AAAA
ATOM	223	C	VAL	A	28	37.363	44.609	53.511	1.00	23.70	AAAA
ATOM	224	O	VAL	A	28	37.943	45.156	54.455	1.00	22.62	AAAA
ATOM	225	N	SER	A	29	37.538	44.989	52.253	1.00	24.27	AAAA
ATOM	226	CA	SER	A	29	38.444	46.082	51.910	1.00	26.03	AAAA
ATOM	227	CB	SER	A	29	38.632	46.178	50.381	1.00	25.95	AAAA
ATOM	228	OG	SER	A	29	37.395	46.417	49.716	1.00	27.57	AAAA
ATOM	229	C	SER	A	29	37.793	47.354	52.440	1.00	25.52	AAAA
ATOM	230	O	SER	A	29	38.463	48.311	52.828	1.00	25.49	AAAA
ATOM	231	N	LEU	A	30	36.468	47.342	52.448	1.00	26.09	AAAA
ATOM	232	CA	LEU	A	30	35.692	48.471	52.926	1.00	26.39	AAAA
ATOM	233	CB	LEU	A	30	34.262	48.365	52.393	1.00	25.89	AAAA
ATOM	234	CG	LEU	A	30	33.265	49.470	52.755	1.00	27.15	AAAA
ATOM	235	CD1	LEU	A	30	32.486	49.101	53.999	1.00	26.34	AAAA
ATOM	236	CD2	LEU	A	30	34.015	50.813	52.897	1.00	25.81	AAAA
ATOM	237	C	LEU	A	30	35.713	48.534	54.453	1.00	26.26	AAAA
ATOM	238	O	LEU	A	30	35.731	49.612	55.037	1.00	27.50	AAAA
ATOM	239	N	LEU	A	31	35.730	47.379	55.097	1.00	25.57	AAAA
ATOM	240	CA	LEU	A	31	35.776	47.343	56.545	1.00	26.87	AAAA
ATOM	241	CB	LEU	A	31	35.752	45.900	57.029	1.00	27.28	AAAA
ATOM	242	CG	LEU	A	31	35.135	45.563	58.383	1.00	27.87	AAAA
ATOM	243	CD1	LEU	A	31	35.855	44.313	58.906	1.00	27.01	AAAA
ATOM	244	CD2	LEU	A	31	35.261	46.706	59.372	1.00	26.32	AAAA
ATOM	245	C	LEU	A	31	37.087	48.003	57.012	1.00	28.08	AAAA
ATOM	246	O	LEU	A	31	37.094	48.854	57.901	1.00	27.42	AAAA
ATOM	247	N	LEU	A	32	38.197	47.584	56.409	1.00	29.52	AAAA
ATOM	248	CA	LEU	A	32	39.508	48.121	56.750	1.00	30.96	AAAA
ATOM	249	CB	LEU	A	32	40.607	47.394	55.950	1.00	31.58	AAAA
ATOM	250	CG	LEU	A	32	40.792	45.904	56.293	1.00	31.63	AAAA
ATOM	251	CD1	LEU	A	32	41.810	45.246	55.380	1.00	31.31	AAAA
ATOM	252	CD2	LEU	A	32	41.232	45.780	57.743	1.00	32.23	AAAA
ATOM	253	C	LEU	A	32	39.599	49.635	56.543	1.00	31.59	AAAA
ATOM	254	O	LEU	A	32	40.081	50.345	57.416	1.00	31.70	AAAA
ATOM	255	N	ARG	A	33	39.140	50.129	55.398	1.00	32.72	AAAA
ATOM	256	CA	ARG	A	33	39.178	51.564	55.141	1.00	33.91	AAAA
ATOM	257	CB	ARG	A	33	38.643	51.903	53.743	1.00	35.10	AAAA
ATOM	258	CG	ARG	A	33	39.627	51.609	52.621	1.00	37.84	AAAA
ATOM	259	CD	ARG	A	33	39.310	52.412	51.374	1.00	39.33	AAAA
ATOM	260	NE	ARG	A	33	38.255	51.806	50.580	1.00	42.51	AAAA
ATOM	261	CZ	ARG	A	33	37.662	52.395	49.541	1.00	44.22	AAAA
ATOM	262	NH1	ARG	A	33	38.016	53.617	49.163	1.00	44.61	AAAA
ATOM	263	NH2	ARG	A	33	36.723	51.752	48.861	1.00	45.23	AAAA
ATOM	264	C	ARG	A	33	38.352	52.305	56.168	1.00	33.48	AAAA

220/263 Figure 19-5

ATOM	265	O	ARG	A	33	38.713	53.390	56.592	1.00	33.61	AAAA
ATOM	266	N	PHE	A	34	37.247	51.682	56.562	1.00	33.78	AAAA
ATOM	267	CA	PHE	A	34	36.292	52.233	57.517	1.00	33.79	AAAA
ATOM	268	CB	PHE	A	34	35.065	51.310	57.573	1.00	33.88	AAAA
ATOM	269	CG	PHE	A	34	33.925	51.840	58.405	1.00	33.16	AAAA
ATOM	270	CD1	PHE	A	34	33.108	52.856	57.925	1.00	32.77	AAAA
ATOM	271	CD2	PHE	A	34	33.668	51.315	59.672	1.00	33.05	AAAA
ATOM	272	CE1	PHE	A	34	32.044	53.343	58.695	1.00	32.86	AAAA
ATOM	273	CE2	PHE	A	34	32.607	51.797	60.454	1.00	33.07	AAAA
ATOM	274	CZ	PHE	A	34	31.794	52.809	59.966	1.00	32.58	AAAA
ATOM	275	C	PHE	A	34	36.881	52.414	58.918	1.00	34.01	AAAA
ATOM	276	O	PHE	A	34	36.903	53.524	59.455	1.00	33.49	AAAA
ATOM	277	N	LYS	A	35	37.350	51.324	59.516	1.00	34.00	AAAA
ATOM	278	CA	LYS	A	35	37.928	51.401	60.843	1.00	33.90	AAAA
ATOM	279	CB	LYS	A	35	38.230	50.010	61.362	1.00	34.07	AAAA
ATOM	280	CG	LYS	A	35	37.000	49.190	61.662	1.00	33.94	AAAA
ATOM	281	CD	LYS	A	35	37.414	47.810	62.106	1.00	35.31	AAAA
ATOM	282	CE	LYS	A	35	38.062	47.072	60.948	1.00	35.91	AAAA
ATOM	283	NZ	LYS	A	35	39.058	47.928	60.236	1.00	36.19	AAAA
ATOM	284	C	LYS	A	35	39.185	52.255	60.881	1.00	34.19	AAAA
ATOM	285	O	LYS	A	35	39.554	52.775	61.929	1.00	34.32	AAAA
ATOM	286	N	ASP	A	36	39.853	52.384	59.745	1.00	33.99	AAAA
ATOM	287	CA	ASP	A	36	41.034	53.216	59.680	1.00	35.17	AAAA
ATOM	288	CB	ASP	A	36	41.812	52.943	58.388	1.00	37.40	AAAA
ATOM	289	CG	ASP	A	36	42.964	53.908	58.186	1.00	38.64	AAAA
ATOM	290	OD1	ASP	A	36	43.648	54.218	59.184	1.00	40.02	AAAA
ATOM	291	OD2	ASP	A	36	43.201	54.341	57.035	1.00	38.74	AAAA
ATOM	292	C	ASP	A	36	40.568	54.670	59.724	1.00	35.85	AAAA
ATOM	293	O	ASP	A	36	41.231	55.527	60.306	1.00	36.88	AAAA
ATOM	294	N	ALA	A	37	39.420	54.940	59.111	1.00	34.96	AAAA
ATOM	295	CA	ALA	A	37	38.851	56.280	59.108	1.00	34.47	AAAA
ATOM	296	CB	ALA	A	37	37.751	56.373	58.067	1.00	33.80	AAAA
ATOM	297	C	ALA	A	37	38.291	56.617	60.499	1.00	34.66	AAAA
ATOM	298	O	ALA	A	37	38.268	57.779	60.899	1.00	34.55	AAAA
ATOM	299	N	MET	A	38	37.830	55.600	61.226	1.00	34.24	AAAA
ATOM	300	CA	MET	A	38	37.287	55.794	62.572	1.00	33.07	AAAA
ATOM	301	CB	MET	A	38	36.289	54.687	62.917	1.00	32.82	AAAA
ATOM	302	CG	MET	A	38	35.084	54.559	61.996	1.00	32.72	AAAA
ATOM	303	SD	MET	A	38	33.980	55.948	62.101	1.00	33.65	AAAA
ATOM	304	CE	MET	A	38	33.550	55.878	63.849	1.00	33.77	AAAA
ATOM	305	C	MET	A	38	38.430	55.724	63.583	1.00	33.12	AAAA
ATOM	306	O	MET	A	38	38.226	55.930	64.777	1.00	32.82	AAAA
ATOM	307	N	ASN	A	39	39.628	55.428	63.090	1.00	32.64	AAAA
ATOM	308	CA	ASN	A	39	40.805	55.266	63.935	1.00	32.38	AAAA
ATOM	309	CB	ASN	A	39	41.200	56.600	64.589	1.00	32.93	AAAA
ATOM	310	CG	ASN	A	39	41.393	57.736	63.571	1.00	34.40	AAAA
ATOM	311	OD1	ASN	A	39	42.180	57.624	62.630	1.00	34.98	AAAA
ATOM	312	ND2	ASN	A	39	40.677	58.838	63.772	1.00	33.52	AAAA
ATOM	313	C	ASN	A	39	40.483	54.212	65.009	1.00	31.69	AAAA
ATOM	314	O	ASN	A	39	40.565	54.490	66.205	1.00	31.12	AAAA
ATOM	315	N	LEU	A	40	40.095	53.010	64.570	1.00	31.76	AAAA
ATOM	316	CA	LEU	A	40	39.750	51.898	65.474	1.00	32.48	AAAA
ATOM	317	CB	LEU	A	40	38.259	51.559	65.386	1.00	32.55	AAAA
ATOM	318	CG	LEU	A	40	37.231	52.581	65.879	1.00	32.84	AAAA
ATOM	319	CD1	LEU	A	40	35.837	52.089	65.554	1.00	33.79	AAAA
ATOM	320	CD2	LEU	A	40	37.372	52.798	67.376	1.00	32.45	AAAA
ATOM	321	C	LEU	A	40	40.555	50.628	65.187	1.00	32.92	AAAA
ATOM	322	O	LEU	A	40	40.196	49.530	65.618	1.00	31.64	AAAA
ATOM	323	N	ILE	A	41	41.652	50.794	64.464	1.00	34.12	AAAA
ATOM	324	CA	ILE	A	41	42.508	49.680	64.116	1.00	36.07	AAAA
ATOM	325	CB	ILE	A	41	42.017	48.991	62.811	1.00	35.51	AAAA
ATOM	326	CG	ILE	A	41	42.070	49.952	61.636	1.00	33.37	AAAA
ATOM	327	CG1	ILE	A	41	42.898	47.790	62.480	1.00	35.97	AAAA
ATOM	328	CD1	ILE	A	41	42.854	46.701	63.500	1.00	37.19	AAAA
ATOM	329	C	ILE	A	41	43.921	50.226	63.916	1.00	38.85	AAAA
ATOM	330	O	ILE	A	41	44.106	51.346	63.413	1.00	38.98	AAAA

221/263

Figure 19-6

ATOM	331	N	ASP	A	42	44.914	49.446	64.329	1.00	40.61	AAAA
ATOM	332	CA	ASP	A	42	46.309	49.843	64.181	1.00	42.57	AAAA
ATOM	333	CB	ASP	A	42	46.973	50.021	65.553	1.00	42.42	AAAA
ATOM	334	CG	ASP	A	42	46.316	51.110	66.381	1.00	42.27	AAAA
ATOM	335	OD1	ASP	A	42	46.227	52.250	65.883	1.00	41.20	AAAA
ATOM	336	OD2	ASP	A	42	45.891	50.833	67.526	1.00	43.36	AAAA
ATOM	337	C	ASP	A	42	47.011	48.752	63.392	1.00	44.05	AAAA
ATOM	338	O	ASP	A	42	46.525	47.620	63.333	1.00	44.88	AAAA
ATOM	339	N	GLU	A	43	48.147	49.090	62.789	1.00	45.10	AAAA
ATOM	340	CA	GLU	A	43	48.905	48.141	61.980	1.00	46.11	AAAA
ATOM	341	CB	GLU	A	43	50.172	48.796	61.454	1.00	46.89	AAAA
ATOM	342	CG	GLU	A	43	49.924	50.057	60.668	1.00	49.30	AAAA
ATOM	343	CD	GLU	A	43	51.187	50.580	60.028	1.00	49.67	AAAA
ATOM	344	OE1	GLU	A	43	51.760	49.839	59.201	1.00	50.60	AAAA
ATOM	345	OE2	GLU	A	43	51.601	51.714	60.349	1.00	49.60	AAAA
ATOM	346	C	GLU	A	43	49.290	46.859	62.701	1.00	46.27	AAAA
ATOM	347	O	GLU	A	43	49.214	45.773	62.131	1.00	46.00	AAAA
ATOM	348	N	LYS	A	44	49.708	46.986	63.954	1.00	46.52	AAAA
ATOM	349	CA	LYS	A	44	50.135	45.832	64.730	1.00	46.31	AAAA
ATOM	350	CB	LYS	A	44	50.762	46.306	66.048	1.00	48.16	AAAA
ATOM	351	CG	LYS	A	44	51.977	47.215	65.799	1.00	51.59	AAAA
ATOM	352	CD	LYS	A	44	52.641	47.734	67.071	1.00	52.87	AAAA
ATOM	353	CE	LYS	A	44	53.851	48.601	66.727	1.00	53.34	AAAA
ATOM	354	NZ	LYS	A	44	54.615	49.033	67.936	1.00	53.45	AAAA
ATOM	355	C	LYS	A	44	49.029	44.828	64.996	1.00	44.74	AAAA
ATOM	356	O	LYS	A	44	49.296	43.735	65.480	1.00	45.35	AAAA
ATOM	357	N	GLU	A	45	47.793	45.190	64.659	1.00	42.49	AAAA
ATOM	358	CA	GLU	A	45	46.638	44.320	64.894	1.00	40.54	AAAA
ATOM	359	CB	GLU	A	45	45.493	45.125	65.517	1.00	40.55	AAAA
ATOM	360	CG	GLU	A	45	45.788	45.731	66.882	1.00	38.87	AAAA
ATOM	361	CD	GLU	A	45	44.663	46.618	67.360	1.00	37.57	AAAA
ATOM	362	OE1	GLU	A	45	44.383	47.631	66.693	1.00	36.29	AAAA
ATOM	363	OE2	GLU	A	45	44.056	46.300	68.399	1.00	38.44	AAAA
ATOM	364	C	GLU	A	45	46.126	43.648	63.630	1.00	39.15	AAAA
ATOM	365	O	GLU	A	45	45.301	42.737	63.681	1.00	39.29	AAAA
ATOM	366	N	LEU	A	46	46.619	44.115	62.497	1.00	37.62	AAAA
ATOM	367	CA	LEU	A	46	46.219	43.589	61.211	1.00	35.88	AAAA
ATOM	368	CB	LEU	A	46	46.125	44.750	60.229	1.00	36.09	AAAA
ATOM	369	CG	LEU	A	46	45.608	44.550	58.817	1.00	36.50	AAAA
ATOM	370	CD1	LEU	A	46	44.182	44.021	58.843	1.00	36.66	AAAA
ATOM	371	CD2	LEU	A	46	45.646	45.893	58.113	1.00	35.85	AAAA
ATOM	372	C	LEU	A	46	47.211	42.542	60.714	1.00	34.97	AAAA
ATOM	373	O	LEU	A	46	48.424	42.670	60.900	1.00	35.72	AAAA
ATOM	374	N	ILE	A	47	46.680	41.484	60.118	1.00	33.25	AAAA
ATOM	375	CA	ILE	A	47	47.497	40.411	59.560	1.00	30.92	AAAA
ATOM	376	CB	ILE	A	47	47.144	39.024	60.167	1.00	31.22	AAAA
ATOM	377	CG2	ILE	A	47	48.093	37.970	59.640	1.00	28.55	AAAA
ATOM	378	CG1	ILE	A	47	47.220	39.063	61.694	1.00	32.04	AAAA
ATOM	379	CD1	ILE	A	47	48.596	39.241	62.242	1.00	34.13	AAAA
ATOM	380	C	ILE	A	47	47.138	40.381	58.076	1.00	29.70	AAAA
ATOM	381	O	ILE	A	47	45.956	40.373	57.714	1.00	28.42	AAAA
ATOM	382	N	LYS	A	48	48.150	40.380	57.221	1.00	28.78	AAAA
ATOM	383	CA	LYS	A	48	47.920	40.349	55.784	1.00	28.42	AAAA
ATOM	384	CB	LYS	A	48	49.203	40.727	55.055	1.00	27.53	AAAA
ATOM	385	CG	LYS	A	48	49.116	40.695	53.556	1.00	28.97	AAAA
ATOM	386	CD	LYS	A	48	50.464	41.104	52.941	1.00	29.67	AAAA
ATOM	387	CE	LYS	A	48	50.493	40.893	51.432	1.00	29.41	AAAA
ATOM	388	NZ	LYS	A	48	49.409	41.645	50.764	1.00	29.68	AAAA
ATOM	389	C	LYS	A	48	47.449	38.950	55.375	1.00	27.81	AAAA
ATOM	390	O	LYS	A	48	48.024	37.938	55.787	1.00	27.96	AAAA
ATOM	391	N	SER	A	49	46.385	38.892	54.581	1.00	26.82	AAAA
ATOM	392	CA	SER	A	49	45.854	37.611	54.141	1.00	26.41	AAAA
ATOM	393	CB	SER	A	49	44.514	37.795	53.420	1.00	25.40	AAAA
ATOM	394	CG	SER	A	49	43.541	38.349	54.276	1.00	25.58	AAAA
ATOM	395	C	SER	A	49	46.814	36.891	53.207	1.00	26.03	AAAA
ATOM	396	O	SER	A	49	47.462	37.513	52.373	1.00	26.98	AAAA

222/263 Figure 19-7

ATOM	397	N	ARG	A	50	46.910	35.576	53.354	1.00	25.51	AAAA
ATOM	398	CA	ARG	A	50	47.755	34.794	52.474	1.00	25.45	AAAA
ATOM	399	CB	ARG	A	50	48.807	33.985	53.252	1.00	25.85	AAAA
ATOM	400	CG	ARG	A	50	48.229	32.819	54.009	1.00	27.16	AAAA
ATOM	401	CD	ARG	A	50	49.280	31.995	54.720	1.00	27.57	AAAA
ATOM	402	NE	ARG	A	50	48.673	30.896	55.482	1.00	27.90	AAAA
ATOM	403	CZ	ARG	A	50	48.106	29.820	54.946	1.00	28.34	AAAA
ATOM	404	NH1	ARG	A	50	48.055	29.672	53.630	1.00	28.19	AAAA
ATOM	405	NH2	ARG	A	50	47.592	28.884	55.735	1.00	28.62	AAAA
ATOM	406	C	ARG	A	50	46.806	33.834	51.762	1.00	24.91	AAAA
ATOM	407	O	ARG	A	50	45.740	33.510	52.283	1.00	23.57	AAAA
ATOM	408	N	PRO	A	51	47.172	33.392	50.549	1.00	24.28	AAAA
ATOM	409	CD	PRO	A	51	48.361	33.761	49.770	1.00	24.13	AAAA
ATOM	410	CA	PRO	A	51	46.355	32.462	49.776	1.00	24.18	AAAA
ATOM	411	CB	PRO	A	51	47.012	32.512	48.390	1.00	24.24	AAAA
ATOM	412	CG	PRO	A	51	47.766	33.862	48.405	1.00	24.11	AAAA
ATOM	413	C	PRO	A	51	46.473	31.070	50.393	1.00	23.69	AAAA
ATOM	414	O	PRO	A	51	47.545	30.680	50.839	1.00	24.13	AAAA
ATOM	415	N	ALA	A	52	45.381	30.325	50.422	1.00	23.36	AAAA
ATOM	416	CA	ALA	A	52	45.419	28.972	50.952	1.00	23.64	AAAA
ATOM	417	CB	ALA	A	52	44.012	28.405	51.029	1.00	23.86	AAAA
ATOM	418	C	ALA	A	52	46.260	28.145	49.994	1.00	23.58	AAAA
ATOM	419	O	ALA	A	52	46.240	28.383	48.806	1.00	24.52	AAAA
ATOM	420	N	THR	A	53	47.009	27.185	50.501	1.00	24.41	AAAA
ATOM	421	CA	THR	A	53	47.815	26.352	49.628	1.00	26.26	AAAA
ATOM	422	CB	THR	A	53	48.933	25.642	50.405	1.00	26.37	AAAA
ATOM	423	OG1	THR	A	53	48.355	24.763	51.375	1.00	26.51	AAAA
ATOM	424	CG2	THR	A	53	49.810	26.648	51.106	1.00	24.48	AAAA
ATOM	425	C	THR	A	53	46.889	25.299	49.034	1.00	27.63	AAAA
ATOM	426	O	THR	A	53	45.870	24.982	49.620	1.00	29.22	AAAA
ATOM	427	N	LYS	A	54	47.240	24.776	47.867	1.00	29.31	AAAA
ATOM	428	CA	LYS	A	54	46.450	23.752	47.189	1.00	30.61	AAAA
ATOM	429	CB	LYS	A	54	47.249	23.182	46.015	1.00	31.68	AAAA
ATOM	430	CG	LYS	A	54	46.585	22.020	45.304	1.00	34.38	AAAA
ATOM	431	CD	LYS	A	54	45.449	22.464	44.417	1.00	36.00	AAAA
ATOM	432	CE	LYS	A	54	45.943	22.850	43.025	1.00	37.55	AAAA
ATOM	433	NZ	LYS	A	54	46.425	21.664	42.236	1.00	37.57	AAAA
ATOM	434	C	LYS	A	54	46.127	22.640	48.170	1.00	31.26	AAAA
ATOM	435	O	LYS	A	54	45.025	22.097	48.176	1.00	31.72	AAAA
ATOM	436	N	GLU	A	55	47.102	22.312	49.006	1.00	31.88	AAAA
ATOM	437	CA	GLU	A	55	46.961	21.260	50.011	1.00	32.29	AAAA
ATOM	438	CB	GLU	A	55	48.266	21.089	50.778	1.00	34.43	AAAA
ATOM	439	CG	GLU	A	55	48.265	19.901	51.706	1.00	38.39	AAAA
ATOM	440	CD	GLU	A	55	49.513	19.839	52.584	1.00	41.46	AAAA
ATOM	441	OE1	GLU	A	55	49.745	18.770	53.200	1.00	43.30	AAAA
ATOM	442	OE2	GLU	A	55	50.245	20.859	52.672	1.00	42.45	AAAA
ATOM	443	C	GLU	A	55	45.851	21.555	51.013	1.00	30.43	AAAA
ATOM	444	O	GLU	A	55	45.048	20.681	51.332	1.00	30.59	AAAA
ATOM	445	N	GLU	A	56	45.822	22.782	51.517	1.00	28.23	AAAA
ATOM	446	CA	GLU	A	56	44.812	23.164	52.488	1.00	27.69	AAAA
ATOM	447	CB	GLU	A	56	45.078	24.588	52.989	1.00	27.90	AAAA
ATOM	448	CG	GLU	A	56	46.434	24.721	53.670	1.00	26.64	AAAA
ATOM	449	CD	GLU	A	56	46.769	26.135	54.098	1.00	26.35	AAAA
ATOM	450	OE1	GLU	A	56	46.615	27.057	53.265	1.00	25.12	AAAA
ATOM	451	OE2	GLU	A	56	47.213	26.315	55.255	1.00	25.70	AAAA
ATOM	452	C	GLU	A	56	43.408	23.043	51.914	1.00	26.99	AAAA
ATOM	453	O	GLU	A	56	42.495	22.574	52.588	1.00	26.25	AAAA
ATOM	454	N	LEU	A	57	43.252	23.447	50.659	1.00	27.26	AAAA
ATOM	455	CA	LEU	A	57	41.965	23.389	49.967	1.00	27.17	AAAA
ATOM	456	CB	LEU	A	57	42.077	24.063	48.596	1.00	26.62	AAAA
ATOM	457	CG	LEU	A	57	42.491	25.545	48.656	1.00	27.64	AAAA
ATOM	458	CD1	LEU	A	57	42.770	26.108	47.269	1.00	26.66	AAAA
ATOM	459	CD2	LEU	A	57	41.389	26.341	49.349	1.00	26.92	AAAA
ATOM	460	C	LEU	A	57	41.552	21.946	49.796	1.00	27.26	AAAA
ATOM	461	O	LEU	A	57	40.363	21.612	49.816	1.00	27.53	AAAA
ATOM	462	N	LEU	A	58	42.547	21.085	49.641	1.00	27.42	AAAA

223/263 Figure 19-8

ATOM	463	CA	LEU	A	58	42.293	19.675	49.457	1.00	26.10	AAAA
ATOM	464	CB	LEU	A	58	43.486	19.019	48.794	1.00	25.43	AAAA
ATOM	465	CG	LEU	A	58	43.623	19.577	47.385	1.00	26.66	AAAA
ATOM	466	CD1	LEU	A	58	44.760	18.884	46.705	1.00	27.12	AAAA
ATOM	467	CD2	LEU	A	58	42.334	19.355	46.600	1.00	26.43	AAAA
ATOM	468	C	LEU	A	58	41.938	18.956	50.731	1.00	25.79	AAAA
ATOM	469	O	LEU	A	58	41.648	17.763	50.692	1.00	26.50	AAAA
ATOM	470	N	LEU	A	59	41.977	19.666	51.858	1.00	24.91	AAAA
ATOM	471	CA	LEU	A	59	41.595	19.070	53.136	1.00	25.15	AAAA
ATOM	472	CB	LEU	A	59	41.958	19.991	54.322	1.00	25.44	AAAA
ATOM	473	CG	LEU	A	59	43.423	20.280	54.710	1.00	24.67	AAAA
ATOM	474	CD1	LEU	A	59	43.502	21.461	55.652	1.00	23.70	AAAA
ATOM	475	CD2	LEU	A	59	44.044	19.044	55.357	1.00	24.08	AAAA
ATOM	476	C	LEU	A	59	40.074	18.870	53.090	1.00	25.41	AAAA
ATOM	477	O	LEU	A	59	39.503	18.266	53.993	1.00	25.88	AAAA
ATOM	478	N	PHE	A	60	39.436	19.392	52.031	1.00	25.05	AAAA
ATOM	479	CA	PHE	A	60	37.983	19.276	51.823	1.00	24.11	AAAA
ATOM	480	CB	PHE	A	60	37.250	20.476	52.440	1.00	21.80	AAAA
ATOM	481	CG	PHE	A	60	35.778	20.534	52.098	1.00	20.07	AAAA
ATOM	482	CD1	PHE	A	60	34.917	19.501	52.462	1.00	19.27	AAAA
ATOM	483	CD2	PHE	A	60	35.249	21.628	51.399	1.00	19.82	AAAA
ATOM	484	CE1	PHE	A	60	33.550	19.557	52.136	1.00	19.26	AAAA
ATOM	485	CE2	PHE	A	60	33.890	21.688	51.071	1.00	17.45	AAAA
ATOM	486	C2	PHE	A	60	33.042	20.652	51.440	1.00	17.92	AAAA
ATOM	487	C	PHE	A	60	37.557	19.139	50.345	1.00	24.02	AAAA
ATOM	488	O	PHE	A	60	36.846	18.201	49.974	1.00	23.27	AAAA
ATOM	489	N	HIS	A	61	37.982	20.079	49.511	1.00	24.40	AAAA
ATOM	490	CA	HIS	A	61	37.626	20.053	48.099	1.00	25.04	AAAA
ATOM	491	CB	HIS	A	61	37.768	21.449	47.494	1.00	24.19	AAAA
ATOM	492	CG	HIS	A	61	36.744	22.429	47.979	1.00	24.44	AAAA
ATOM	493	CD2	HIS	A	61	35.429	22.559	47.683	1.00	24.12	AAAA
ATOM	494	ND1	HIS	A	61	37.038	23.444	48.864	1.00	24.36	AAAA
ATOM	495	CE1	HIS	A	61	35.952	24.159	49.089	1.00	23.18	AAAA
ATOM	496	NE2	HIS	A	61	34.962	23.643	48.385	1.00	23.91	AAAA
ATOM	497	C	HIS	A	61	38.416	19.054	47.253	1.00	25.60	AAAA
ATOM	498	O	HIS	A	61	39.596	18.805	47.498	1.00	26.94	AAAA
ATOM	499	N	THR	A	62	37.754	18.496	46.244	1.00	26.68	AAAA
ATOM	500	CA	THR	A	62	38.369	17.522	45.333	1.00	28.17	AAAA
ATOM	501	CB	THR	A	62	37.290	16.695	44.614	1.00	28.15	AAAA
ATOM	502	OG1	THR	A	62	36.544	17.541	43.731	1.00	28.10	AAAA
ATOM	503	CG2	THR	A	62	36.334	16.094	45.629	1.00	28.24	AAAA
ATOM	504	C	THR	A	62	39.226	18.217	44.278	1.00	29.28	AAAA
ATOM	505	O	THR	A	62	38.876	19.286	43.792	1.00	29.52	AAAA
ATOM	506	N	GLU	A	63	40.344	17.606	43.912	1.00	31.33	AAAA
ATOM	507	CA	GLU	A	63	41.249	18.202	42.928	1.00	32.42	AAAA
ATOM	508	CB	GLU	A	63	42.333	17.219	42.536	1.00	34.37	AAAA
ATOM	509	CG	GLU	A	63	43.304	16.869	43.609	1.00	37.20	AAAA
ATOM	510	CD	GLU	A	63	44.427	16.022	43.052	1.00	38.79	AAAA
ATOM	511	OE1	GLU	A	63	45.100	16.499	42.097	1.00	37.96	AAAA
ATOM	512	OE2	GLU	A	63	44.619	14.892	43.564	1.00	39.68	AAAA
ATOM	513	C	GLU	A	63	40.607	18.687	41.639	1.00	31.96	AAAA
ATOM	514	O	GLU	A	63	40.824	19.816	41.215	1.00	32.10	AAAA
ATOM	515	N	ASP	A	64	39.845	17.814	40.998	1.00	31.52	AAAA
ATOM	516	CA	ASP	A	64	39.204	18.165	39.753	1.00	31.36	AAAA
ATOM	517	CB	ASP	A	64	38.301	17.018	39.295	1.00	33.99	AAAA
ATOM	518	CG	ASP	A	64	37.213	16.694	40.302	1.00	37.38	AAAA
ATOM	519	OD1	ASP	A	64	36.375	15.801	40.027	1.00	39.80	AAAA
ATOM	520	OD2	ASP	A	64	37.188	17.332	41.374	1.00	38.67	AAAA
ATOM	521	C	ASP	A	64	38.412	19.465	39.902	1.00	30.02	AAAA
ATOM	522	O	ASP	A	64	38.462	20.331	39.026	1.00	30.47	AAAA
ATOM	523	N	TYR	A	65	37.695	19.608	41.012	1.00	27.51	AAAA
ATOM	524	CA	TYR	A	65	36.918	20.814	41.248	1.00	26.03	AAAA
ATOM	525	CB	TYR	A	65	36.010	20.654	42.467	1.00	25.42	AAAA
ATOM	526	CG	TYR	A	65	35.339	21.946	42.866	1.00	24.90	AAAA
ATOM	527	CD1	TYR	A	65	34.525	22.636	41.964	1.00	25.04	AAAA
ATOM	528	CE1	TYR	A	65	33.914	23.823	42.308	1.00	25.01	AAAA

224/263

Figure 19-9

ATOM	529	CD2	TYR	A	55	35.525	22.486	44.136	1.00	24.65	AAAA
ATOM	530	CE2	TYR	A	55	34.920	23.677	44.497	1.00	25.86	AAAA
ATOM	531	CZ	TYR	A	55	34.110	24.349	43.576	1.00	26.69	AAAA
ATOM	532	OH	TYR	A	55	33.499	25.543	43.924	1.00	27.20	AAAA
ATOM	533	C	TYR	A	55	37.814	22.022	41.464	1.00	24.91	AAAA
ATOM	534	O	TYR	A	55	37.460	23.129	41.096	1.00	25.62	AAAA
ATOM	535	N	ILE	A	56	38.965	21.812	42.080	1.00	23.20	AAAA
ATOM	536	CA	ILE	A	56	39.877	22.902	42.328	1.00	22.33	AAAA
ATOM	537	CB	ILE	A	56	40.924	22.520	43.402	1.00	21.45	AAAA
ATOM	538	CG2	ILE	A	56	41.927	23.652	43.617	1.00	20.00	AAAA
ATOM	539	CG1	ILE	A	56	40.220	22.289	44.729	1.00	20.16	AAAA
ATOM	540	CD1	ILE	A	56	39.528	23.523	45.228	1.00	19.68	AAAA
ATOM	541	C	ILE	A	56	40.558	23.261	41.023	1.00	22.68	AAAA
ATOM	542	O	ILE	A	56	40.636	24.425	40.665	1.00	23.19	AAAA
ATOM	543	N	ASN	A	57	41.036	22.262	40.295	1.00	22.96	AAAA
ATOM	544	CA	ASN	A	57	41.698	22.545	39.029	1.00	23.92	AAAA
ATOM	545	CB	ASN	A	57	42.292	21.261	38.395	1.00	24.24	AAAA
ATOM	546	CG	ASN	A	57	43.344	20.588	39.289	1.00	23.38	AAAA
ATOM	547	OD1	ASN	A	57	44.196	21.256	39.859	1.00	23.47	AAAA
ATOM	548	ND2	ASN	A	57	43.290	19.258	39.392	1.00	23.20	AAAA
ATOM	549	C	ASN	A	57	40.717	23.216	38.063	1.00	23.82	AAAA
ATOM	550	O	ASN	A	57	41.123	23.996	37.204	1.00	24.63	AAAA
ATOM	551	N	THR	A	58	39.427	22.928	38.213	1.00	24.08	AAAA
ATOM	552	CA	THR	A	58	38.428	23.534	37.343	1.00	25.28	AAAA
ATOM	553	CB	THR	A	58	37.030	22.904	37.525	1.00	24.55	AAAA
ATOM	554	OG1	THR	A	58	37.090	21.500	37.258	1.00	24.64	AAAA
ATOM	555	CG2	THR	A	58	36.049	23.534	36.564	1.00	23.58	AAAA
ATOM	556	C	THR	A	58	38.322	25.023	37.664	1.00	26.31	AAAA
ATOM	557	O	THR	A	58	38.114	25.854	36.771	1.00	26.69	AAAA
ATOM	558	N	LEU	A	59	38.462	25.351	38.945	1.00	26.59	AAAA
ATOM	559	CA	LEU	A	59	38.381	26.729	39.378	1.00	27.05	AAAA
ATOM	560	CB	LEU	A	59	38.321	26.807	40.904	1.00	27.15	AAAA
ATOM	561	CG	LEU	A	59	37.003	26.397	41.551	1.00	25.68	AAAA
ATOM	562	CD1	LEU	A	59	37.088	26.491	43.062	1.00	26.30	AAAA
ATOM	563	CD2	LEU	A	59	35.933	27.316	41.044	1.00	26.14	AAAA
ATOM	564	C	LEU	A	59	39.570	27.508	38.867	1.00	28.44	AAAA
ATOM	565	O	LEU	A	59	39.425	28.619	38.356	1.00	28.59	AAAA
ATOM	566	N	MET	A	70	40.748	26.914	39.009	1.00	29.31	AAAA
ATOM	567	CA	MET	A	70	41.981	27.536	38.571	1.00	29.89	AAAA
ATOM	568	CB	MET	A	70	43.160	26.692	39.044	1.00	31.04	AAAA
ATOM	569	CG	MET	A	70	43.164	26.528	40.562	1.00	31.79	AAAA
ATOM	570	SD	MET	A	70	44.608	25.684	41.183	1.00	32.58	AAAA
ATOM	571	CE	MET	A	70	45.859	26.820	40.670	1.00	30.82	AAAA
ATOM	572	C	MET	A	70	42.017	27.723	37.057	1.00	30.36	AAAA
ATOM	573	O	MET	A	70	42.462	28.769	36.559	1.00	30.18	AAAA
ATOM	574	N	GLU	A	71	41.538	26.719	36.328	1.00	30.34	AAAA
ATOM	575	CA	GLU	A	71	41.519	26.795	34.874	1.00	30.73	AAAA
ATOM	576	CB	GLU	A	71	41.140	25.442	34.266	1.00	33.47	AAAA
ATOM	577	CG	GLU	A	71	41.122	25.430	32.731	1.00	37.11	AAAA
ATOM	578	CD	GLU	A	71	42.513	25.676	32.093	1.00	40.49	AAAA
ATOM	579	OE1	GLU	A	71	42.570	25.798	30.844	1.00	41.95	AAAA
ATOM	580	OE2	GLU	A	71	43.541	25.738	32.825	1.00	40.74	AAAA
ATOM	581	C	GLU	A	71	40.537	27.851	34.392	1.00	29.78	AAAA
ATOM	582	O	GLU	A	71	40.852	28.642	33.508	1.00	27.82	AAAA
ATOM	583	N	ALA	A	72	39.352	27.855	34.992	1.00	29.85	AAAA
ATOM	584	CA	ALA	A	72	38.296	28.790	34.635	1.00	29.88	AAAA
ATOM	585	CB	ALA	A	72	37.022	28.432	35.374	1.00	29.07	AAAA
ATOM	586	C	ALA	A	72	38.667	30.238	34.907	1.00	30.78	AAAA
ATOM	587	O	ALA	A	72	38.359	31.122	34.108	1.00	31.27	AAAA
ATOM	588	N	GLU	A	73	39.336	30.491	36.023	1.00	31.07	AAAA
ATOM	589	CA	GLU	A	73	39.710	31.856	36.346	1.00	31.65	AAAA
ATOM	590	CB	GLU	A	73	40.243	31.954	37.785	1.00	30.52	AAAA
ATOM	591	CG	GLU	A	73	40.643	33.370	38.198	1.00	28.73	AAAA
ATOM	592	CD	GLU	A	73	41.076	33.484	39.651	1.00	28.77	AAAA
ATOM	593	OE1	GLU	A	73	40.239	33.260	40.546	1.00	28.94	AAAA
ATOM	594	OE2	GLU	A	73	42.258	33.795	39.906	1.00	28.57	AAAA

225/263 Figure 19-10

ATOM	595	C	GLU	A	73	40.726	32.461	35.378	1.00	33.54	AAAA
ATOM	596	O	GLU	A	73	40.456	33.499	34.767	1.00	34.93	AAAA
ATOM	597	N	ARG	A	74	41.885	31.832	35.214	1.00	34.35	AAAA
ATOM	598	CA	ARG	A	74	42.890	32.428	34.334	1.00	36.04	AAAA
ATOM	599	CB	ARG	A	74	44.238	31.710	34.482	1.00	36.92	AAAA
ATOM	600	CG	ARG	A	74	44.327	30.313	33.923	1.00	36.14	AAAA
ATOM	601	CD	ARG	A	74	45.508	29.589	34.543	1.00	39.55	AAAA
ATOM	602	NE	ARG	A	74	45.893	28.404	33.785	1.00	42.02	AAAA
ATOM	603	CZ	ARG	A	74	46.632	28.436	32.675	1.00	42.69	AAAA
ATOM	604	NH1	ARG	A	74	47.071	29.593	32.191	1.00	42.76	AAAA
ATOM	605	NH2	ARG	A	74	46.933	27.309	32.046	1.00	42.92	AAAA
ATOM	606	C	ARG	A	74	42.476	32.532	32.864	1.00	36.56	AAAA
ATOM	607	O	ARG	A	74	42.842	33.493	32.187	1.00	37.73	AAAA
ATOM	608	N	SER	A	75	41.711	31.567	32.367	1.00	36.60	AAAA
ATOM	609	CA	SER	A	75	41.248	31.622	30.987	1.00	36.82	AAAA
ATOM	610	CB	SER	A	75	40.916	30.218	30.478	1.00	36.10	AAAA
ATOM	611	OG	SER	A	75	39.736	29.723	31.083	1.00	36.39	AAAA
ATOM	612	C	SER	A	75	39.980	32.476	31.001	1.00	36.90	AAAA
ATOM	613	O	SER	A	75	39.401	32.791	29.963	1.00	36.25	AAAA
ATOM	614	N	GLN	A	76	39.568	32.845	32.208	1.00	37.62	AAAA
ATOM	615	CA	GLN	A	76	38.368	33.639	32.427	1.00	37.92	AAAA
ATOM	616	CB	GLN	A	76	38.613	35.100	32.049	1.00	38.23	AAAA
ATOM	617	CG	GLN	A	76	37.630	36.048	32.717	1.00	40.67	AAAA
ATOM	618	CD	GLN	A	76	37.929	36.298	34.199	1.00	41.40	AAAA
ATOM	619	OE1	GLN	A	76	38.226	35.379	34.973	1.00	40.79	AAAA
ATOM	620	NE2	GLN	A	76	37.833	37.556	34.597	1.00	42.32	AAAA
ATOM	621	C	GLN	A	76	37.223	33.064	31.600	1.00	37.75	AAAA
ATOM	622	O	GLN	A	76	36.521	33.789	30.901	1.00	38.13	AAAA
ATOM	623	N	SER	A	77	37.045	31.749	31.685	1.00	37.52	AAAA
ATOM	624	CA	SER	A	77	35.990	31.061	30.950	1.00	37.75	AAAA
ATOM	625	CB	SER	A	77	36.537	30.440	29.664	1.00	37.90	AAAA
ATOM	626	OG	SER	A	77	36.851	31.441	28.724	1.00	40.32	AAAA
ATOM	627	C	SER	A	77	35.338	29.960	31.757	1.00	37.55	AAAA
ATOM	628	O	SER	A	77	35.790	29.620	32.846	1.00	36.81	AAAA
ATOM	629	N	VAL	A	78	34.264	29.412	31.198	1.00	37.82	AAAA
ATOM	630	CA	VAL	A	78	33.538	28.309	31.812	1.00	37.99	AAAA
ATOM	631	CB	VAL	A	78	32.027	28.514	31.715	1.00	37.19	AAAA
ATOM	632	CG1	VAL	A	78	31.310	27.439	32.497	1.00	36.84	AAAA
ATOM	633	CG2	VAL	A	78	31.662	29.906	32.201	1.00	37.60	AAAA
ATOM	634	C	VAL	A	78	33.918	27.089	30.976	1.00	38.28	AAAA
ATOM	635	O	VAL	A	78	33.497	26.959	29.819	1.00	39.18	AAAA
ATOM	636	N	PRO	A	79	34.734	26.187	31.537	1.00	37.69	AAAA
ATOM	637	CD	PRO	A	79	35.347	26.167	32.869	1.00	37.65	AAAA
ATOM	638	CA	PRO	A	79	35.146	24.998	30.797	1.00	37.54	AAAA
ATOM	639	CB	PRO	A	79	36.127	24.325	31.759	1.00	37.45	AAAA
ATOM	640	CG	PRO	A	79	36.655	25.489	32.557	1.00	37.65	AAAA
ATOM	641	C	PRO	A	79	33.980	24.089	30.434	1.00	37.20	AAAA
ATOM	642	O	PRO	A	79	32.958	24.050	31.120	1.00	36.43	AAAA
ATOM	643	N	LYS	A	80	34.154	23.363	29.338	1.00	37.42	AAAA
ATOM	644	CA	LYS	A	80	33.160	22.423	28.855	1.00	37.35	AAAA
ATOM	645	CB	LYS	A	80	33.757	21.586	27.725	1.00	37.99	AAAA
ATOM	646	CG	LYS	A	80	32.928	20.379	27.280	1.00	38.94	AAAA
ATOM	647	CD	LYS	A	80	31.835	20.710	26.286	1.00	39.07	AAAA
ATOM	648	CE	LYS	A	80	31.320	19.402	25.688	1.00	40.43	AAAA
ATOM	649	NZ	LYS	A	80	30.498	19.543	24.450	1.00	40.48	AAAA
ATOM	650	C	LYS	A	80	32.752	21.515	30.003	1.00	36.85	AAAA
ATOM	651	O	LYS	A	80	33.610	20.942	30.676	1.00	36.56	AAAA
ATOM	652	N	GLY	A	81	31.443	21.408	30.217	1.00	35.94	AAAA
ATOM	653	CA	GLY	A	81	30.903	20.570	31.268	1.00	35.48	AAAA
ATOM	654	C	GLY	A	81	31.110	21.054	32.695	1.00	35.23	AAAA
ATOM	655	O	GLY	A	81	30.749	20.355	33.644	1.00	35.46	AAAA
ATOM	656	N	ALA	A	82	31.677	22.241	32.867	1.00	35.17	AAAA
ATOM	657	CA	ALA	A	82	31.919	22.743	34.213	1.00	35.02	AAAA
ATOM	658	CB	ALA	A	82	33.076	23.743	34.208	1.00	35.13	AAAA
ATOM	659	C	ALA	A	82	30.674	23.378	34.797	1.00	34.39	AAAA
ATOM	660	O	ALA	A	82	30.451	23.332	36.001	1.00	33.82	AAAA

226/263 Figure 19-11

ATOM	661	N	ARG	A	83	29.858	23.960	33.932	1.00	34.77	AAAA
ATOM	662	CA	ARG	A	83	28.637	24.613	34.361	1.00	35.34	AAAA
ATOM	663	CB	ARG	A	83	27.899	25.180	33.150	1.00	36.26	AAAA
ATOM	664	CG	ARG	A	83	27.045	26.395	33.464	1.00	37.09	AAAA
ATOM	665	CD	ARG	A	83	26.209	26.141	34.686	1.00	37.48	AAAA
ATOM	666	NE	ARG	A	83	25.475	27.310	35.134	1.00	37.35	AAAA
ATOM	667	CZ	ARG	A	83	24.711	27.311	36.218	1.00	37.77	AAAA
ATOM	668	NH1	ARG	A	83	24.606	26.204	36.940	1.00	37.29	AAAA
ATOM	669	NH2	ARG	A	83	24.040	28.401	36.568	1.00	38.34	AAAA
ATOM	670	C	ARG	A	83	27.739	23.603	35.065	1.00	36.30	AAAA
ATOM	671	O	ARG	A	83	27.232	23.854	36.154	1.00	36.17	AAAA
ATOM	672	N	GLU	A	84	27.565	22.450	34.431	1.00	37.19	AAAA
ATOM	673	CA	GLU	A	84	26.721	21.382	34.948	1.00	37.80	AAAA
ATOM	674	CB	GLU	A	84	26.466	20.375	33.833	1.00	40.55	AAAA
ATOM	675	CG	GLU	A	84	25.643	19.171	34.232	1.00	43.12	AAAA
ATOM	676	CD	GLU	A	84	25.362	18.268	33.046	1.00	44.98	AAAA
ATOM	677	OE1	GLU	A	84	24.573	17.301	33.195	1.00	46.36	AAAA
ATOM	678	OE2	GLU	A	84	25.937	18.532	31.962	1.00	44.94	AAAA
ATOM	679	C	GLU	A	84	27.290	20.657	36.158	1.00	37.07	AAAA
ATOM	680	O	GLU	A	84	26.642	20.555	37.199	1.00	36.17	AAAA
ATOM	681	N	LYS	A	85	28.506	20.152	35.999	1.00	36.23	AAAA
ATOM	682	CA	LYS	A	85	29.202	19.412	37.043	1.00	35.36	AAAA
ATOM	683	CB	LYS	A	85	30.449	18.761	36.437	1.00	36.96	AAAA
ATOM	684	CG	LYS	A	85	31.394	18.158	37.465	1.00	39.04	AAAA
ATOM	685	CD	LYS	A	85	30.995	16.766	37.919	1.00	40.59	AAAA
ATOM	686	CE	LYS	A	85	31.508	15.719	36.933	1.00	41.88	AAAA
ATOM	687	NZ	LYS	A	85	32.998	15.817	36.757	1.00	42.00	AAAA
ATOM	688	C	LYS	A	85	29.620	20.202	38.289	1.00	33.86	AAAA
ATOM	689	O	LYS	A	85	29.576	19.679	39.404	1.00	33.82	AAAA
ATOM	690	N	TYR	A	86	30.014	21.458	38.097	1.00	32.06	AAAA
ATOM	691	CA	TYR	A	86	30.514	22.279	39.194	1.00	29.44	AAAA
ATOM	692	CB	TYR	A	86	31.956	22.683	38.875	1.00	29.97	AAAA
ATOM	693	CG	TYR	A	86	32.872	21.496	38.621	1.00	29.99	AAAA
ATOM	694	CD1	TYR	A	86	33.281	20.666	39.666	1.00	29.24	AAAA
ATOM	695	CE1	TYR	A	86	34.126	19.582	39.437	1.00	29.85	AAAA
ATOM	696	CD2	TYR	A	86	33.329	21.204	37.329	1.00	30.16	AAAA
ATOM	697	CE2	TYR	A	86	34.173	20.118	37.087	1.00	29.61	AAAA
ATOM	698	CZ	TYR	A	86	34.570	19.313	38.148	1.00	29.79	AAAA
ATOM	699	OH	TYR	A	86	35.414	18.253	37.923	1.00	29.48	AAAA
ATOM	700	C	TYR	A	86	29.705	23.509	39.572	1.00	27.81	AAAA
ATOM	701	O	TYR	A	86	30.052	24.202	40.524	1.00	27.56	AAAA
ATOM	702	N	ASN	A	87	28.642	23.784	38.828	1.00	26.60	AAAA
ATOM	703	CA	ASN	A	87	27.777	24.924	39.111	1.00	26.56	AAAA
ATOM	704	CB	ASN	A	87	27.172	24.772	40.508	1.00	26.39	AAAA
ATOM	705	CG	ASN	A	87	25.863	25.544	40.684	1.00	26.64	AAAA
ATOM	706	OD1	ASN	A	87	25.335	25.632	41.790	1.00	26.84	AAAA
ATOM	707	ND2	ASN	A	87	25.330	26.084	39.597	1.00	26.33	AAAA
ATOM	708	C	ASN	A	87	28.587	26.217	39.024	1.00	26.40	AAAA
ATOM	709	O	ASN	A	87	28.430	27.129	39.832	1.00	24.80	AAAA
ATOM	710	N	ILE	A	88	29.448	26.273	38.015	1.00	27.57	AAAA
ATOM	711	CA	ILE	A	88	30.330	27.409	37.767	1.00	27.88	AAAA
ATOM	712	CB	ILE	A	88	31.817	26.932	37.648	1.00	27.38	AAAA
ATOM	713	CG2	ILE	A	88	32.684	27.994	36.986	1.00	26.34	AAAA
ATOM	714	CG1	ILE	A	88	32.354	26.543	39.026	1.00	28.35	AAAA
ATOM	715	CD1	ILE	A	88	32.356	27.671	40.042	1.00	27.78	AAAA
ATOM	716	C	ILE	A	88	29.946	28.110	36.472	1.00	29.17	AAAA
ATOM	717	O	ILE	A	88	29.530	27.469	35.515	1.00	29.75	AAAA
ATOM	718	N	GLY	A	89	30.092	29.429	36.443	1.00	29.96	AAAA
ATOM	719	CA	GLY	A	89	29.791	30.162	35.229	1.00	30.24	AAAA
ATOM	720	C	GLY	A	89	28.430	30.805	35.242	1.00	30.44	AAAA
ATOM	721	O	GLY	A	89	28.177	31.769	34.514	1.00	31.14	AAAA
ATOM	722	N	GLY	A	90	27.542	30.268	36.061	1.00	30.00	AAAA
ATOM	723	CA	GLY	A	90	26.221	30.841	36.129	1.00	30.52	AAAA
ATOM	724	C	GLY	A	90	26.283	32.262	36.661	1.00	31.09	AAAA
ATOM	725	O	GLY	A	90	27.356	32.795	36.962	1.00	30.34	AAAA
ATOM	726	N	TYR	A	91	25.112	32.873	36.768	1.00	31.09	AAAA

227/263 Figure 19-12

ATOM	727	CA	TYR	A	91	24.977	34.213	37.290	1.00	31.27	AAAA
ATOM	728	CB	TYR	A	91	23.515	34.634	37.195	1.00	31.82	AAAA
ATOM	729	CG	TYR	A	91	23.169	35.825	38.047	1.00	31.81	AAAA
ATOM	730	CD1	TYR	A	91	23.536	37.108	37.670	1.00	32.44	AAAA
ATOM	731	CE1	TYR	A	91	23.250	38.203	38.475	1.00	31.88	AAAA
ATOM	732	CD2	TYR	A	91	22.505	35.663	39.254	1.00	32.63	AAAA
ATOM	733	CE2	TYR	A	91	22.215	36.754	40.068	1.00	32.60	AAAA
ATOM	734	CZ	TYR	A	91	22.589	38.016	39.668	1.00	31.59	AAAA
ATOM	735	OH	TYR	A	91	22.283	39.094	40.450	1.00	31.94	AAAA
ATOM	736	C	TYR	A	91	25.384	34.202	38.753	1.00	31.56	AAAA
ATOM	737	O	TYR	A	91	26.075	35.105	39.233	1.00	31.21	AAAA
ATOM	738	N	GLU	A	92	24.925	33.158	39.438	1.00	31.51	AAAA
ATOM	739	CA	GLU	A	92	25.143	32.941	40.865	1.00	32.70	AAAA
ATOM	740	CB	GLU	A	92	24.463	31.626	41.268	1.00	33.55	AAAA
ATOM	741	CG	GLU	A	92	24.174	31.495	42.747	1.00	34.16	AAAA
ATOM	742	CD	GLU	A	92	23.311	30.278	43.087	1.00	35.31	AAAA
ATOM	743	OE1	GLU	A	92	23.857	29.148	43.152	1.00	34.30	AAAA
ATOM	744	OE2	GLU	A	92	22.076	30.466	43.275	1.00	35.36	AAAA
ATOM	745	C	GLU	A	92	26.619	32.902	41.248	1.00	33.02	AAAA
ATOM	746	O	GLU	A	92	27.073	33.623	42.140	1.00	32.91	AAAA
ATOM	747	N	ASN	A	93	27.358	32.049	40.550	1.00	32.84	AAAA
ATOM	748	CA	ASN	A	93	28.785	31.861	40.777	1.00	31.92	AAAA
ATOM	749	CB	ASN	A	93	29.015	30.437	41.278	1.00	31.18	AAAA
ATOM	750	CG	ASN	A	93	27.948	29.994	42.259	1.00	30.34	AAAA
ATOM	751	OD1	ASN	A	93	27.723	30.642	43.271	1.00	31.20	AAAA
ATOM	752	ND2	ASN	A	93	27.284	28.892	41.955	1.00	29.02	AAAA
ATOM	753	C	ASN	A	93	29.442	32.052	39.411	1.00	30.84	AAAA
ATOM	754	O	ASN	A	93	29.823	31.082	38.758	1.00	30.82	AAAA
ATOM	755	N	PRO	A	94	29.605	33.309	38.975	1.00	29.56	AAAA
ATOM	756	CD	PRO	A	94	29.312	34.590	39.626	1.00	29.03	AAAA
ATOM	757	CA	PRO	A	94	30.209	33.564	37.671	1.00	28.89	AAAA
ATOM	758	CB	PRO	A	94	29.890	35.045	37.416	1.00	28.22	AAAA
ATOM	759	CG	PRO	A	94	28.839	35.377	38.435	1.00	29.50	AAAA
ATOM	760	C	PRO	A	94	31.698	33.351	37.664	1.00	28.25	AAAA
ATOM	761	O	PRO	A	94	32.308	32.996	38.671	1.00	28.21	AAAA
ATOM	762	N	VAL	A	95	32.257	33.593	36.488	1.00	27.36	AAAA
ATOM	763	CA	VAL	A	95	33.676	33.530	36.247	1.00	26.24	AAAA
ATOM	764	CB	VAL	A	95	33.945	33.289	34.741	1.00	26.10	AAAA
ATOM	765	CG1	VAL	A	95	35.373	33.717	34.357	1.00	25.47	AAAA
ATOM	766	CG2	VAL	A	95	33.736	31.826	34.434	1.00	25.59	AAAA
ATOM	767	C	VAL	A	95	34.178	34.919	36.647	1.00	26.56	AAAA
ATOM	768	O	VAL	A	95	33.560	35.937	36.307	1.00	27.18	AAAA
ATOM	769	N	SER	A	96	35.280	34.966	37.382	1.00	25.23	AAAA
ATOM	770	CA	SER	A	96	35.858	36.237	37.790	1.00	24.51	AAAA
ATOM	771	CB	SER	A	96	34.935	36.961	38.774	1.00	23.22	AAAA
ATOM	772	OG	SER	A	96	34.941	36.297	40.014	1.00	19.76	AAAA
ATOM	773	C	SER	A	96	37.169	35.920	38.485	1.00	24.84	AAAA
ATOM	774	O	SER	A	96	37.590	34.764	38.530	1.00	25.97	AAAA
ATOM	775	N	TYR	A	97	37.824	36.933	39.030	1.00	24.02	AAAA
ATOM	776	CA	TYR	A	97	39.047	36.664	39.744	1.00	24.55	AAAA
ATOM	777	CB	TYR	A	97	40.071	37.762	39.504	1.00	23.94	AAAA
ATOM	778	CG	TYR	A	97	40.682	37.636	38.128	1.00	23.72	AAAA
ATOM	779	CD1	TYR	A	97	40.177	38.341	37.039	1.00	23.11	AAAA
ATOM	780	CE1	TYR	A	97	40.700	38.136	35.758	1.00	23.50	AAAA
ATOM	781	CD2	TYR	A	97	41.717	36.735	37.903	1.00	22.25	AAAA
ATOM	782	CE2	TYR	A	97	42.236	36.526	36.640	1.00	22.86	AAAA
ATOM	783	CD	TYR	A	97	41.730	37.217	35.572	1.00	23.56	AAAA
ATOM	784	CH	TYR	A	97	42.232	36.941	34.318	1.00	24.06	AAAA
ATOM	785	C	TYR	A	97	38.800	36.436	41.228	1.00	25.08	AAAA
ATOM	786	O	TYR	A	97	39.739	36.266	42.009	1.00	26.91	AAAA
ATOM	787	N	ALA	A	98	37.522	36.406	41.589	1.00	24.73	AAAA
ATOM	788	CA	ALA	A	98	37.083	36.159	42.951	1.00	24.50	AAAA
ATOM	789	CB	ALA	A	98	35.800	36.925	43.235	1.00	24.48	AAAA
ATOM	790	C	ALA	A	98	36.824	34.661	43.088	1.00	23.95	AAAA
ATOM	791	O	ALA	A	98	36.929	34.100	44.171	1.00	24.21	AAAA
ATOM	792	N	MET	A	99	36.502	34.011	41.976	1.00	23.10	AAAA

228/263 Figure 19-13

ATOM	793	CA	MET	A	99	36.208	32.584	42.000	1.00	22.61	AAAA
ATOM	794	CB	MET	A	99	35.855	32.089	40.597	1.00	23.25	AAAA
ATOM	795	CG	MET	A	99	37.009	32.063	39.607	1.00	23.22	AAAA
ATOM	796	SD	MET	A	99	36.360	31.808	37.952	1.00	25.21	AAAA
ATOM	797	CE	MET	A	99	35.328	30.374	38.258	1.00	22.04	AAAA
ATOM	798	C	MET	A	99	37.319	31.720	42.581	1.00	21.80	AAAA
ATOM	799	O	MET	A	99	37.052	30.695	43.199	1.00	21.29	AAAA
ATOM	800	N	PHE	A	100	38.567	32.111	42.380	1.00	21.87	AAAA
ATOM	801	CA	PHE	A	100	39.650	31.322	42.936	1.00	21.11	AAAA
ATOM	802	CB	PHE	A	100	40.388	30.552	41.841	1.00	20.25	AAAA
ATOM	803	CG	PHE	A	100	41.451	29.648	42.375	1.00	20.14	AAAA
ATOM	804	CD1	PHE	A	100	41.114	28.462	43.010	1.00	20.49	AAAA
ATOM	805	CD2	PHE	A	100	42.785	30.050	42.373	1.00	19.82	AAAA
ATOM	806	CE1	PHE	A	100	42.090	27.695	43.646	1.00	19.54	AAAA
ATOM	807	CE2	PHE	A	100	43.755	29.300	43.001	1.00	19.22	AAAA
ATOM	808	CZ	PHE	A	100	43.410	28.122	43.641	1.00	19.47	AAAA
ATOM	809	C	PHE	A	100	40.649	32.161	43.743	1.00	21.37	AAAA
ATOM	810	O	PHE	A	100	40.959	31.822	44.887	1.00	21.26	AAAA
ATOM	811	N	THR	A	101	41.142	33.252	43.161	1.00	20.94	AAAA
ATOM	812	CA	THR	A	101	42.119	34.097	43.847	1.00	21.95	AAAA
ATOM	813	CB	THR	A	101	42.691	35.181	42.905	1.00	22.21	AAAA
ATOM	814	OG1	THR	A	101	43.511	34.552	41.917	1.00	22.90	AAAA
ATOM	815	CG2	THR	A	101	43.535	36.186	43.667	1.00	21.38	AAAA
ATOM	816	C	THR	A	101	41.584	34.755	45.117	1.00	22.60	AAAA
ATOM	817	O	THR	A	101	42.248	34.723	46.147	1.00	23.38	AAAA
ATOM	818	N	GLY	A	102	40.394	35.343	45.049	1.00	22.13	AAAA
ATOM	819	CA	GLY	A	102	39.826	35.972	46.227	1.00	22.03	AAAA
ATOM	820	C	GLY	A	102	39.340	34.928	47.221	1.00	21.36	AAAA
ATOM	821	O	GLY	A	102	39.433	35.104	48.439	1.00	20.02	AAAA
ATOM	822	N	SER	A	103	38.816	33.833	46.677	1.00	21.86	AAAA
ATOM	823	CA	SER	A	103	38.311	32.719	47.466	1.00	21.68	AAAA
ATOM	824	CB	SER	A	103	37.699	31.668	46.557	1.00	21.56	AAAA
ATOM	825	OG	SER	A	103	36.604	32.216	45.857	1.00	23.67	AAAA
ATOM	826	C	SER	A	103	39.450	32.098	48.229	1.00	22.67	AAAA
ATOM	827	O	SER	A	103	39.314	31.806	49.412	1.00	22.44	AAAA
ATOM	828	N	SER	A	104	40.578	31.898	47.545	1.00	23.37	AAAA
ATOM	829	CA	SER	A	104	41.746	31.305	48.183	1.00	23.50	AAAA
ATOM	830	CB	SER	A	104	42.862	31.070	47.172	1.00	24.80	AAAA
ATOM	831	OG	SER	A	104	42.441	30.169	46.175	1.00	28.38	AAAA
ATOM	832	C	SER	A	104	42.254	32.230	49.256	1.00	22.79	AAAA
ATOM	833	O	SER	A	104	42.707	31.794	50.307	1.00	22.66	AAAA
ATOM	834	N	LEU	A	105	42.160	33.518	48.970	1.00	22.08	AAAA
ATOM	835	CA	LEU	A	105	42.626	34.541	49.870	1.00	21.70	AAAA
ATOM	836	CB	LEU	A	105	42.524	35.882	49.159	1.00	21.89	AAAA
ATOM	837	CG	LEU	A	105	43.332	37.038	49.718	1.00	23.64	AAAA
ATOM	838	CD1	LEU	A	105	44.830	36.692	49.639	1.00	22.01	AAAA
ATOM	839	CD2	LEU	A	105	43.004	38.304	48.919	1.00	23.60	AAAA
ATOM	840	C	LEU	A	105	41.767	34.525	51.131	1.00	22.29	AAAA
ATOM	841	O	LEU	A	105	42.277	34.595	52.249	1.00	21.95	AAAA
ATOM	842	N	ALA	A	106	40.458	34.429	50.934	1.00	22.23	AAAA
ATOM	843	CA	ALA	A	106	39.515	34.394	52.042	1.00	22.32	AAAA
ATOM	844	CB	ALA	A	106	38.068	34.472	51.526	1.00	22.05	AAAA
ATOM	845	C	ALA	A	106	39.704	33.126	52.840	1.00	21.99	AAAA
ATOM	846	O	ALA	A	106	39.578	33.145	54.061	1.00	23.18	AAAA
ATOM	847	N	THR	A	107	40.011	32.032	52.144	1.00	21.24	AAAA
ATOM	848	CA	THR	A	107	40.209	30.732	52.779	1.00	20.60	AAAA
ATOM	849	CB	THR	A	107	40.170	29.571	51.749	1.00	19.82	AAAA
ATOM	850	OG1	THR	A	107	38.903	29.553	51.083	1.00	18.56	AAAA
ATOM	851	CG2	THR	A	107	40.360	28.242	52.455	1.00	18.58	AAAA
ATOM	852	C	THR	A	107	41.516	30.630	53.561	1.00	21.41	AAAA
ATOM	853	O	THR	A	107	41.537	30.040	54.646	1.00	23.16	AAAA
ATOM	854	N	GLY	A	108	42.601	31.176	53.003	1.00	20.14	AAAA
ATOM	855	CA	GLY	A	108	43.878	31.145	53.684	1.00	18.20	AAAA
ATOM	856	C	GLY	A	108	43.739	31.933	54.972	1.00	18.43	AAAA
ATOM	857	O	GLY	A	108	44.335	31.600	55.998	1.00	17.52	AAAA
ATOM	858	N	SER	A	109	42.909	32.969	54.929	1.00	18.56	AAAA

229/263 Figure 19-14

ATOM	859	CA	SER	A	109	42.683	33.805	56.098	1.00	19.67	AAAA
ATOM	860	CB	SER	A	109	41.899	35.058	55.707	1.00	20.27	AAAA
ATOM	861	OG	SER	A	109	42.618	35.803	54.746	1.00	21.80	AAAA
ATOM	862	C	SER	A	109	41.955	33.066	57.219	1.00	19.61	AAAA
ATOM	863	O	SER	A	109	42.078	33.426	58.388	1.00	18.40	AAAA
ATOM	864	N	THR	A	110	41.186	32.042	56.866	1.00	19.88	AAAA
ATOM	865	CA	THR	A	110	40.493	31.288	57.891	1.00	20.51	AAAA
ATOM	866	CB	THR	A	110	39.365	30.438	57.304	1.00	20.62	AAAA
ATOM	867	OG1	THR	A	110	38.236	31.284	57.050	1.00	20.80	AAAA
ATOM	868	CG2	THR	A	110	38.974	29.313	58.262	1.00	20.53	AAAA
ATOM	869	C	THR	A	110	41.504	30.420	58.601	1.00	20.36	AAAA
ATOM	870	O	THR	A	110	41.455	30.268	59.822	1.00	20.78	AAAA
ATOM	871	N	VAL	A	111	42.431	29.855	57.832	1.00	20.85	AAAA
ATOM	872	CA	VAL	A	111	43.480	29.053	58.423	1.00	21.03	AAAA
ATOM	873	CB	VAL	A	111	44.318	28.323	57.345	1.00	21.05	AAAA
ATOM	874	CG1	VAL	A	111	45.537	27.644	57.983	1.00	19.91	AAAA
ATOM	875	CG2	VAL	A	111	43.460	27.281	56.648	1.00	18.39	AAAA
ATOM	876	C	VAL	A	111	44.374	30.005	59.232	1.00	21.84	AAAA
ATOM	877	O	VAL	A	111	44.825	29.671	60.331	1.00	22.73	AAAA
ATOM	878	N	GLN	A	112	44.612	31.204	58.712	1.00	21.62	AAAA
ATOM	879	CA	GLN	A	112	45.449	32.133	59.452	1.00	21.89	AAAA
ATOM	880	CB	GLN	A	112	45.630	33.450	58.690	1.00	22.50	AAAA
ATOM	881	CG	GLN	A	112	46.288	33.283	57.335	1.00	23.68	AAAA
ATOM	882	CD	GLN	A	112	46.414	34.578	56.569	1.00	23.18	AAAA
ATOM	883	OE1	GLN	A	112	47.389	35.310	56.722	1.00	23.86	AAAA
ATOM	884	NE2	GLN	A	112	45.413	34.879	55.752	1.00	21.90	AAAA
ATOM	885	C	GLN	A	112	44.766	32.383	60.774	1.00	21.84	AAAA
ATOM	886	O	GLN	A	112	45.389	32.316	61.835	1.00	22.47	AAAA
ATOM	887	N	ALA	A	113	43.468	32.651	60.700	1.00	21.34	AAAA
ATOM	888	CA	ALA	A	113	42.682	32.934	61.884	1.00	20.84	AAAA
ATOM	889	CB	ALA	A	113	41.244	33.172	61.504	1.00	18.52	AAAA
ATOM	890	C	ALA	A	113	42.795	31.782	62.865	1.00	21.75	AAAA
ATOM	891	O	ALA	A	113	42.880	31.985	64.084	1.00	22.24	AAAA
ATOM	892	N	ILE	A	114	42.797	30.569	62.329	1.00	22.54	AAAA
ATOM	893	CA	ILE	A	114	42.891	29.393	63.160	1.00	23.16	AAAA
ATOM	894	CB	ILE	A	114	42.557	28.146	62.352	1.00	23.33	AAAA
ATOM	895	CG2	ILE	A	114	42.939	26.912	63.106	1.00	23.80	AAAA
ATOM	896	CG1	ILE	A	114	41.058	28.130	62.047	1.00	23.48	AAAA
ATOM	897	CD1	ILE	A	114	40.610	26.951	61.204	1.00	22.08	AAAA
ATOM	898	C	ILE	A	114	44.268	29.270	63.792	1.00	24.33	AAAA
ATOM	899	O	ILE	A	114	44.373	29.013	64.990	1.00	25.30	AAAA
ATOM	900	N	GLU	A	115	45.319	29.490	63.002	1.00	24.96	AAAA
ATOM	901	CA	GLU	A	115	46.699	29.395	63.503	1.00	26.61	AAAA
ATOM	902	CB	GLU	A	115	47.708	29.753	62.406	1.00	24.75	AAAA
ATOM	903	CG	GLU	A	115	47.444	29.033	61.103	1.00	25.80	AAAA
ATOM	904	CD	GLU	A	115	48.471	29.323	60.030	1.00	26.07	AAAA
ATOM	905	OE1	GLU	A	115	48.911	30.484	59.940	1.00	27.15	AAAA
ATOM	906	OE2	GLU	A	115	48.819	28.402	59.260	1.00	25.45	AAAA
ATOM	907	C	GLU	A	115	46.877	30.340	64.680	1.00	27.89	AAAA
ATOM	908	O	GLU	A	115	47.480	29.975	65.695	1.00	28.04	AAAA
ATOM	909	N	GLU	A	116	46.337	31.552	64.531	1.00	29.15	AAAA
ATOM	910	CA	GLU	A	116	46.408	32.579	65.563	1.00	29.42	AAAA
ATOM	911	CB	GLU	A	116	45.751	33.871	65.082	1.00	28.26	AAAA
ATOM	912	CG	GLU	A	116	46.482	34.529	63.945	1.00	28.93	AAAA
ATOM	913	CD	GLU	A	116	47.902	34.937	64.318	1.00	28.32	AAAA
ATOM	914	OE1	GLU	A	116	48.081	35.878	65.123	1.00	27.68	AAAA
ATOM	915	OE2	GLU	A	116	48.838	34.297	63.810	1.00	27.38	AAAA
ATOM	916	C	GLU	A	116	45.737	32.126	66.845	1.00	29.77	AAAA
ATOM	917	O	GLU	A	116	46.338	32.196	67.920	1.00	30.29	AAAA
ATOM	918	N	PHE	A	117	44.492	31.665	66.727	1.00	29.64	AAAA
ATOM	919	CA	PHE	A	117	43.741	31.204	67.887	1.00	29.33	AAAA
ATOM	920	CB	PHE	A	117	42.425	30.552	67.480	1.00	28.89	AAAA
ATOM	921	CG	PHE	A	117	41.604	30.087	68.651	1.00	28.93	AAAA
ATOM	922	CD1	PHE	A	117	41.010	31.010	69.510	1.00	28.42	AAAA
ATOM	923	CD2	PHE	A	117	41.441	28.723	68.910	1.00	29.06	AAAA
ATOM	924	CE1	PHE	A	117	40.261	30.588	70.610	1.00	28.68	AAAA

230/263 Figure 19-15

ATOM	925	CE2	PHE	A	117	40.695	28.284	70.009	1.00	29.16	AAAA
ATOM	926	CZ	PHE	A	117	40.103	29.227	70.862	1.00	29.03	AAAA
ATOM	927	C	PHE	A	117	44.545	30.195	68.671	1.00	29.22	AAAA
ATOM	928	O	PHE	A	117	44.677	30.315	69.884	1.00	30.29	AAAA
ATOM	929	N	LEU	A	118	45.066	29.195	67.965	1.00	29.24	AAAA
ATOM	930	CA	LEU	A	118	45.864	28.145	68.576	1.00	29.50	AAAA
ATOM	931	CB	LEU	A	118	46.182	27.047	67.550	1.00	28.57	AAAA
ATOM	932	CG	LEU	A	118	44.962	26.296	66.989	1.00	28.16	AAAA
ATOM	933	CD1	LEU	A	118	45.421	25.090	66.191	1.00	25.58	AAAA
ATOM	934	CD2	LEU	A	118	44.053	25.846	68.128	1.00	27.64	AAAA
ATOM	935	C	LEU	A	118	47.150	28.649	69.227	1.00	30.14	AAAA
ATOM	936	O	LEU	A	118	47.727	27.954	70.056	1.00	29.94	AAAA
ATOM	937	N	LYS	A	119	47.602	29.845	68.847	1.00	31.36	AAAA
ATOM	938	CA	LYS	A	119	48.798	30.451	69.448	1.00	32.52	AAAA
ATOM	939	CB	LYS	A	119	49.396	31.539	68.559	1.00	32.38	AAAA
ATOM	940	CG	LYS	A	119	49.882	31.108	67.199	1.00	33.03	AAAA
ATOM	941	CD	LYS	A	119	50.371	32.321	66.411	1.00	32.74	AAAA
ATOM	942	CE	LYS	A	119	50.681	31.939	64.972	1.00	33.94	AAAA
ATOM	943	NZ	LYS	A	119	51.125	33.099	64.152	1.00	34.93	AAAA
ATOM	944	C	LYS	A	119	48.385	31.143	70.744	1.00	33.74	AAAA
ATOM	945	O	LYS	A	119	49.218	31.748	71.413	1.00	34.85	AAAA
ATOM	946	N	GLY	A	120	47.096	31.079	71.073	1.00	33.68	AAAA
ATOM	947	CA	GLY	A	120	46.600	31.736	72.263	1.00	33.69	AAAA
ATOM	948	C	GLY	A	120	45.987	33.110	71.988	1.00	34.11	AAAA
ATOM	949	O	GLY	A	120	45.588	33.802	72.932	1.00	33.65	AAAA
ATOM	950	N	ASN	A	121	45.904	33.513	70.717	1.00	33.58	AAAA
ATOM	951	CA	ASN	A	121	45.326	34.820	70.368	1.00	33.35	AAAA
ATOM	952	CB	ASN	A	121	46.194	35.537	69.341	1.00	33.18	AAAA
ATOM	953	CG	ASN	A	121	47.570	35.828	69.859	1.00	34.31	AAAA
ATOM	954	OD1	ASN	A	121	48.333	34.921	70.154	1.00	35.67	AAAA
ATOM	955	ND2	ASN	A	121	47.897	37.096	69.975	1.00	34.18	AAAA
ATOM	956	C	ASN	A	121	43.888	34.805	69.839	1.00	32.85	AAAA
ATOM	957	O	ASN	A	121	43.304	33.751	69.599	1.00	32.78	AAAA
ATOM	958	N	VAL	A	122	43.338	36.003	69.655	1.00	32.47	AAAA
ATOM	959	CA	VAL	A	122	41.980	36.200	69.148	1.00	30.89	AAAA
ATOM	960	CB	VAL	A	122	41.182	37.145	70.070	1.00	31.05	AAAA
ATOM	961	CG1	VAL	A	122	39.831	37.423	69.489	1.00	30.95	AAAA
ATOM	962	CG2	VAL	A	122	41.038	36.516	71.440	1.00	31.19	AAAA
ATOM	963	C	VAL	A	122	42.056	36.805	67.750	1.00	30.19	AAAA
ATOM	964	O	VAL	A	122	42.694	37.840	67.535	1.00	31.28	AAAA
ATOM	965	N	ALA	A	123	41.405	36.147	66.800	1.00	28.62	AAAA
ATOM	966	CA	ALA	A	123	41.415	36.589	65.421	1.00	26.49	AAAA
ATOM	967	CB	ALA	A	123	42.323	35.708	64.599	1.00	26.51	AAAA
ATOM	968	C	ALA	A	123	40.038	36.570	64.836	1.00	25.59	AAAA
ATOM	969	O	ALA	A	123	39.173	35.814	65.252	1.00	26.27	AAAA
ATOM	970	N	PHE	A	124	39.848	37.421	62.847	1.00	25.44	AAAA
ATOM	971	CA	PHE	A	124	38.590	37.534	61.156	1.00	23.87	AAAA
ATOM	972	CB	PHE	A	124	37.832	38.779	61.646	1.00	23.58	AAAA
ATOM	973	CG	PHE	A	124	36.591	39.119	62.841	1.00	23.71	AAAA
ATOM	974	CD1	PHE	A	124	35.668	38.140	62.495	1.00	23.44	AAAA
ATOM	975	CD2	PHE	A	124	36.311	40.449	62.498	1.00	23.75	AAAA
ATOM	976	CE1	PHE	A	124	34.479	38.483	61.823	1.00	23.31	AAAA
ATOM	977	CE2	PHE	A	124	35.131	40.796	61.833	1.00	21.71	AAAA
ATOM	978	CZ	PHE	A	124	34.217	39.815	61.497	1.00	22.35	AAAA
ATOM	979	C	PHE	A	124	38.951	37.673	61.700	1.00	23.26	AAAA
ATOM	980	O	PHE	A	124	39.720	38.555	61.323	1.00	22.29	AAAA
ATOM	981	N	ASN	A	125	38.427	36.759	60.897	1.00	23.24	AAAA
ATOM	982	CA	ASN	A	125	38.622	36.785	59.457	1.00	21.08	AAAA
ATOM	983	CB	ASN	A	125	39.181	35.470	58.951	1.00	19.90	AAAA
ATOM	984	CG	ASN	A	125	39.098	35.360	57.454	1.00	20.64	AAAA
ATOM	985	OD1	ASN	A	125	39.389	36.317	56.748	1.00	21.63	AAAA
ATOM	986	ND2	ASN	A	125	38.721	34.190	56.956	1.00	19.93	AAAA
ATOM	987	C	ASN	A	125	37.269	37.059	58.813	1.00	20.19	AAAA
ATOM	988	O	ASN	A	125	36.469	36.148	58.579	1.00	19.21	AAAA
ATOM	989	N	PRO	A	126	36.991	38.340	58.543	1.00	19.14	AAAA
ATOM	990	CD	PRO	A	126	37.893	39.460	58.858	1.00	19.22	AAAA

231/263 Figure 19-16

ATOM	991	CA	PRO	A	126	35.766	38.849	57.932	1.00	19.52	AAAA
ATOM	992	CB	PRO	A	126	36.005	40.359	57.941	1.00	18.55	AAAA
ATOM	993	CG	PRO	A	126	37.511	40.465	57.799	1.00	17.97	AAAA
ATOM	994	C	PRO	A	126	35.456	38.313	56.526	1.00	19.41	AAAA
ATOM	995	O	PRO	A	126	34.303	38.349	56.080	1.00	19.68	AAAA
ATOM	996	N	ALA	A	127	36.477	37.814	55.835	1.00	18.17	AAAA
ATOM	997	CA	ALA	A	127	36.283	37.314	54.481	1.00	17.66	AAAA
ATOM	998	CB	ALA	A	127	37.547	37.520	53.658	1.00	17.08	AAAA
ATOM	999	C	ALA	A	127	35.875	35.857	54.443	1.00	17.46	AAAA
ATOM	1000	O	ALA	A	127	35.438	35.359	53.409	1.00	18.92	AAAA
ATOM	1001	N	GLY	A	128	36.019	35.180	55.570	1.00	15.94	AAAA
ATOM	1002	CA	GLY	A	128	35.685	33.780	55.642	1.00	15.45	AAAA
ATOM	1003	C	GLY	A	128	34.226	33.593	55.955	1.00	16.08	AAAA
ATOM	1004	O	GLY	A	128	33.485	34.557	55.997	1.00	15.43	AAAA
ATOM	1005	N	GLY	A	129	33.821	32.353	56.198	1.00	16.77	AAAA
ATOM	1006	CA	GLY	A	129	32.426	32.082	56.462	1.00	17.82	AAAA
ATOM	1007	C	GLY	A	129	31.669	31.822	55.169	1.00	18.64	AAAA
ATOM	1008	O	GLY	A	129	30.469	32.051	55.108	1.00	18.48	AAAA
ATOM	1009	N	MET	A	130	32.380	31.368	54.137	1.00	20.45	AAAA
ATOM	1010	CA	MET	A	130	31.790	31.029	52.826	1.00	21.60	AAAA
ATOM	1011	CB	MET	A	130	32.866	31.117	51.744	1.00	22.02	AAAA
ATOM	1012	CG	MET	A	130	33.551	32.472	51.698	1.00	21.75	AAAA
ATOM	1013	SD	MET	A	130	34.971	32.567	50.599	1.00	24.75	AAAA
ATOM	1014	CE	MET	A	130	34.268	32.137	49.048	1.00	24.40	AAAA
ATOM	1015	C	MET	A	130	31.328	29.587	53.002	1.00	22.08	AAAA
ATOM	1016	O	MET	A	130	31.970	28.641	52.546	1.00	22.98	AAAA
ATOM	1017	N	HIS	A	131	30.184	29.452	53.659	1.00	22.25	AAAA
ATOM	1018	CA	HIS	A	131	29.618	28.171	54.062	1.00	20.49	AAAA
ATOM	1019	CB	HIS	A	131	28.832	28.421	55.342	1.00	20.00	AAAA
ATOM	1020	CG	HIS	A	131	27.679	29.360	55.161	1.00	17.93	AAAA
ATOM	1021	CD2	HIS	A	131	27.091	29.846	54.043	1.00	17.88	AAAA
ATOM	1022	ND1	HIS	A	131	26.952	29.854	56.219	1.00	19.33	AAAA
ATOM	1023	CE1	HIS	A	131	25.968	30.607	55.758	1.00	16.99	AAAA
ATOM	1024	NE2	HIS	A	131	26.031	30.617	54.441	1.00	17.43	AAAA
ATOM	1025	C	HIS	A	131	28.763	27.332	53.141	1.00	19.97	AAAA
ATOM	1026	O	HIS	A	131	28.330	26.262	53.541	1.00	19.61	AAAA
ATOM	1027	N	HIS	A	132	28.518	27.796	51.923	1.00	20.11	AAAA
ATOM	1028	CA	HIS	A	132	27.673	27.058	50.994	1.00	17.76	AAAA
ATOM	1029	CB	HIS	A	132	26.879	28.044	50.127	1.00	16.76	AAAA
ATOM	1030	CG	HIS	A	132	25.824	28.815	50.862	1.00	15.35	AAAA
ATOM	1031	CD2	HIS	A	132	25.567	30.146	50.920	1.00	14.15	AAAA
ATOM	1032	ND1	HIS	A	132	24.804	28.200	51.557	1.00	16.15	AAAA
ATOM	1033	CE1	HIS	A	132	23.966	29.119	52.005	1.00	14.13	AAAA
ATOM	1034	NE2	HIS	A	132	24.405	30.307	51.632	1.00	14.65	AAAA
ATOM	1035	C	HIS	A	132	28.355	26.051	50.065	1.00	17.99	AAAA
ATOM	1036	O	HIS	A	132	27.742	25.053	49.684	1.00	18.54	AAAA
ATOM	1037	N	ALA	A	133	29.604	26.305	49.690	1.00	17.82	AAAA
ATOM	1038	CA	ALA	A	133	30.300	25.441	48.742	1.00	18.38	AAAA
ATOM	1039	CB	ALA	A	133	31.684	25.961	48.507	1.00	17.53	AAAA
ATOM	1040	C	ALA	A	133	30.366	23.970	49.130	1.00	20.92	AAAA
ATOM	1041	O	ALA	A	133	30.578	23.633	50.298	1.00	21.79	AAAA
ATOM	1042	N	PHE	A	134	30.184	23.086	48.152	1.00	20.58	AAAA
ATOM	1043	CA	PHE	A	134	30.258	21.663	48.455	1.00	21.38	AAAA
ATOM	1044	CB	PHE	A	134	29.168	20.860	47.731	1.00	19.41	AAAA
ATOM	1045	CG	PHE	A	134	27.772	21.229	48.126	1.00	18.32	AAAA
ATOM	1046	CD1	PHE	A	134	27.027	22.099	47.357	1.00	19.22	AAAA
ATOM	1047	CD2	PHE	A	134	27.193	20.701	49.271	1.00	19.14	AAAA
ATOM	1048	CE1	PHE	A	134	25.714	22.438	47.726	1.00	18.56	AAAA
ATOM	1049	CE2	PHE	A	134	25.889	21.036	49.644	1.00	17.72	AAAA
ATOM	1050	CZ	PHE	A	134	25.158	21.903	48.866	1.00	18.01	AAAA
ATOM	1051	C	PHE	A	134	31.625	21.124	48.081	1.00	22.90	AAAA
ATOM	1052	O	PHE	A	134	32.459	21.833	47.544	1.00	23.37	AAAA
ATOM	1053	N	LYS	A	135	31.842	19.861	48.390	1.00	24.63	AAAA
ATOM	1054	CA	LYS	A	135	33.095	19.195	48.122	1.00	27.16	AAAA
ATOM	1055	CB	LYS	A	135	32.926	17.714	48.480	1.00	28.53	AAAA
ATOM	1056	CG	LYS	A	135	34.133	16.843	48.292	1.00	31.01	AAAA

232/263

Figure 19-17

ATOM	1057	CD	LYS	A	135	33.879	15.472	48.910	1.00	32.75	AAAA
ATOM	1058	CE	LYS	A	135	33.961	15.495	50.457	1.00	33.96	AAAA
ATOM	1059	NZ	LYS	A	135	35.371	15.664	50.976	1.00	33.04	AAAA
ATOM	1060	C	LYS	A	135	33.577	19.390	46.673	1.00	27.37	AAAA
ATOM	1061	O	LYS	A	135	34.769	19.596	46.437	1.00	27.35	AAAA
ATOM	1062	N	SER	A	136	32.658	19.354	45.714	1.00	27.32	AAAA
ATOM	1063	CA	SER	A	136	33.028	19.527	44.313	1.00	28.31	AAAA
ATOM	1064	CB	SER	A	136	33.093	18.162	43.626	1.00	28.56	AAAA
ATOM	1065	OG	SER	A	136	33.822	17.242	44.417	1.00	29.28	AAAA
ATOM	1066	C	SER	A	136	31.993	20.395	43.599	1.00	28.91	AAAA
ATOM	1067	O	SER	A	136	31.568	20.080	42.486	1.00	28.78	AAAA
ATOM	1068	N	ARG	A	137	31.595	21.502	44.212	1.00	29.08	AAAA
ATOM	1069	CA	ARG	A	137	30.574	22.311	43.576	1.00	29.66	AAAA
ATOM	1070	CB	ARG	A	137	29.259	21.528	43.657	1.00	31.65	AAAA
ATOM	1071	CG	ARG	A	137	27.989	22.273	43.355	1.00	33.89	AAAA
ATOM	1072	CD	ARG	A	137	26.862	21.267	43.373	1.00	35.93	AAAA
ATOM	1073	NE	ARG	A	137	26.961	20.366	42.228	1.00	36.31	AAAA
ATOM	1074	CZ	ARG	A	137	26.505	20.660	41.015	1.00	35.99	AAAA
ATOM	1075	NH1	ARG	A	137	25.915	21.834	40.798	1.00	34.63	AAAA
ATOM	1076	NH2	ARG	A	137	26.650	19.786	40.025	1.00	35.35	AAAA
ATOM	1077	C	ARG	A	137	30.402	23.723	44.116	1.00	28.53	AAAA
ATOM	1078	O	ARG	A	137	30.418	23.946	45.324	1.00	28.51	AAAA
ATOM	1079	N	ALA	A	138	30.247	24.673	43.202	1.00	27.53	AAAA
ATOM	1080	CA	ALA	A	138	30.039	26.063	43.581	1.00	27.64	AAAA
ATOM	1081	CB	ALA	A	138	30.236	26.984	42.381	1.00	27.87	AAAA
ATOM	1082	C	ALA	A	138	28.601	26.130	44.079	1.00	27.27	AAAA
ATOM	1083	O	ALA	A	138	27.769	25.321	43.671	1.00	28.30	AAAA
ATOM	1084	N	ASN	A	139	28.292	27.080	44.951	1.00	26.16	AAAA
ATOM	1085	CA	ASN	A	139	26.945	27.134	45.480	1.00	25.39	AAAA
ATOM	1086	CB	ASN	A	139	26.673	25.847	46.282	1.00	24.58	AAAA
ATOM	1087	CG	ASN	A	139	25.343	25.872	47.017	1.00	25.37	AAAA
ATOM	1088	OD1	ASN	A	139	24.272	26.017	46.413	1.00	24.20	AAAA
ATOM	1089	ND2	ASN	A	139	25.408	25.720	48.338	1.00	24.91	AAAA
ATOM	1090	C	ASN	A	139	26.683	28.358	46.341	1.00	24.90	AAAA
ATOM	1091	O	ASN	A	139	27.346	28.570	47.348	1.00	24.98	AAAA
ATOM	1092	N	GLY	A	140	25.702	29.145	45.916	1.00	24.46	AAAA
ATOM	1093	CA	GLY	A	140	25.294	30.336	46.625	1.00	22.96	AAAA
ATOM	1094	C	GLY	A	140	26.383	31.358	46.755	1.00	22.24	AAAA
ATOM	1095	O	GLY	A	140	26.663	31.817	47.867	1.00	23.09	AAAA
ATOM	1096	N	PHE	A	141	26.992	31.711	45.625	1.00	20.60	AAAA
ATOM	1097	CA	PHE	A	141	28.075	32.700	45.572	1.00	19.43	AAAA
ATOM	1098	CB	PHE	A	141	27.758	33.920	46.430	1.00	19.86	AAAA
ATOM	1099	CG	PHE	A	141	26.453	34.577	46.114	1.00	21.18	AAAA
ATOM	1100	CD1	PHE	A	141	25.974	35.592	46.934	1.00	20.49	AAAA
ATOM	1101	CD2	PHE	A	141	25.723	34.218	44.985	1.00	21.42	AAAA
ATOM	1102	CE1	PHE	A	141	24.800	36.242	46.638	1.00	22.45	AAAA
ATOM	1103	CE2	PHE	A	141	24.540	34.859	44.672	1.00	21.76	AAAA
ATOM	1104	CZ	PHE	A	141	24.072	35.881	45.499	1.00	23.05	AAAA
ATOM	1105	C	PHE	A	141	29.396	32.132	46.069	1.00	18.68	AAAA
ATOM	1106	O	PHE	A	141	30.438	32.784	45.944	1.00	19.19	AAAA
ATOM	1107	N	CYS	A	142	29.367	30.930	46.635	1.00	16.93	AAAA
ATOM	1108	CA	CYS	A	142	30.594	30.332	47.150	1.00	16.80	AAAA
ATOM	1109	CB	CYS	A	142	30.323	29.689	48.509	1.00	16.51	AAAA
ATOM	1110	SG	CYS	A	142	29.524	30.826	49.617	1.00	15.01	AAAA
ATOM	1111	C	CYS	A	142	31.227	29.315	46.221	1.00	16.45	AAAA
ATOM	1112	O	CYS	A	142	30.533	28.565	45.556	1.00	15.32	AAAA
ATOM	1113	N	TYR	A	143	32.558	29.311	46.190	1.00	18.39	AAAA
ATOM	1114	CA	TYR	A	143	33.340	28.394	45.362	1.00	18.63	AAAA
ATOM	1115	CB	TYR	A	143	34.298	29.154	44.438	1.00	19.48	AAAA
ATOM	1116	CG	TYR	A	143	33.664	30.214	43.571	1.00	19.55	AAAA
ATOM	1117	CD1	TYR	A	143	33.480	31.510	44.043	1.00	20.27	AAAA
ATOM	1118	CE1	TYR	A	143	32.856	32.473	43.261	1.00	21.63	AAAA
ATOM	1119	CD2	TYR	A	143	33.212	29.910	42.292	1.00	20.14	AAAA
ATOM	1120	CE2	TYR	A	143	32.588	30.863	41.507	1.00	20.82	AAAA
ATOM	1121	CZ	TYR	A	143	32.414	32.135	41.998	1.00	20.90	AAAA
ATOM	1122	OH	TYR	A	143	31.787	33.071	41.228	1.00	23.36	AAAA

233/263 Figure 19-18

ATOM	1123	C	TYR	A	143	34.162	27.490	46.283	1.00	19.06	AAAA
ATOM	1124	O	TYR	A	143	34.319	26.289	46.032	1.00	18.40	AAAA
ATOM	1125	N	ILE	A	144	34.695	28.087	47.344	1.00	19.15	AAAA
ATOM	1126	CA	ILE	A	144	35.490	27.350	48.315	1.00	19.97	AAAA
ATOM	1127	CB	ILE	A	144	36.952	27.861	48.355	1.00	19.74	AAAA
ATOM	1128	CG2	ILE	A	144	37.757	27.088	49.410	1.00	18.03	AAAA
ATOM	1129	CG1	ILE	A	144	37.584	27.671	46.965	1.00	20.12	AAAA
ATOM	1130	CD1	ILE	A	144	39.053	28.072	46.846	1.00	21.05	AAAA
ATOM	1131	C	ILE	A	144	34.833	27.532	49.665	1.00	20.22	AAAA
ATOM	1132	O	ILE	A	144	34.357	28.626	49.981	1.00	19.94	AAAA
ATOM	1133	N	ASN	A	145	34.787	26.451	50.440	1.00	20.57	AAAA
ATOM	1134	CA	ASN	A	145	34.165	26.448	51.770	1.00	20.39	AAAA
ATOM	1135	CB	ASN	A	145	33.450	25.114	51.990	1.00	19.39	AAAA
ATOM	1136	CG	ASN	A	145	32.505	25.143	53.171	1.00	19.31	AAAA
ATOM	1137	OD1	ASN	A	145	32.862	25.583	54.263	1.00	21.26	AAAA
ATOM	1138	ND2	ASN	A	145	31.290	24.667	52.960	1.00	17.08	AAAA
ATOM	1139	C	ASN	A	145	35.236	26.621	52.856	1.00	20.17	AAAA
ATOM	1140	O	ASN	A	145	35.690	25.622	53.421	1.00	19.75	AAAA
ATOM	1141	N	ASN	A	146	35.644	27.862	53.148	1.00	20.06	AAAA
ATOM	1142	CA	ASN	A	146	36.671	28.075	54.166	1.00	20.98	AAAA
ATOM	1143	CB	ASN	A	146	37.019	29.573	54.333	1.00	21.78	AAAA
ATOM	1144	CG	ASN	A	146	35.876	30.411	54.882	1.00	22.78	AAAA
ATOM	1145	OD1	ASN	A	146	35.651	30.465	56.091	1.00	22.83	AAAA
ATOM	1146	ND2	ASN	A	146	35.144	31.078	53.983	1.00	23.70	AAAA
ATOM	1147	C	ASN	A	146	36.307	27.413	55.496	1.00	21.18	AAAA
ATOM	1148	O	ASN	A	146	37.169	26.823	56.139	1.00	21.48	AAAA
ATOM	1149	N	PRO	A	147	35.031	27.476	55.922	1.00	20.88	AAAA
ATOM	1150	CD	PRO	A	147	33.835	28.120	55.358	1.00	21.85	AAAA
ATOM	1151	CA	PRO	A	147	34.674	26.831	57.183	1.00	21.42	AAAA
ATOM	1152	CB	PRO	A	147	33.176	27.073	57.261	1.00	21.00	AAAA
ATOM	1153	CG	PRO	A	147	33.052	28.408	56.605	1.00	20.47	AAAA
ATOM	1154	C	PRO	A	147	35.015	25.334	57.174	1.00	22.79	AAAA
ATOM	1155	O	PRO	A	147	35.650	24.833	58.099	1.00	25.69	AAAA
ATOM	1156	N	ALA	A	148	34.603	24.616	56.136	1.00	22.34	AAAA
ATOM	1157	CA	ALA	A	148	34.889	23.193	56.070	1.00	22.23	AAAA
ATOM	1158	CB	ALA	A	148	34.260	22.561	54.825	1.00	22.87	AAAA
ATOM	1159	C	ALA	A	148	36.378	22.998	56.054	1.00	22.33	AAAA
ATOM	1160	O	ALA	A	148	36.912	22.249	56.861	1.00	23.42	AAAA
ATOM	1161	N	VAL	A	149	37.050	23.661	55.122	1.00	22.50	AAAA
ATOM	1162	CA	VAL	A	149	38.505	23.569	55.018	1.00	21.29	AAAA
ATOM	1163	CB	VAL	A	149	39.066	24.581	54.002	1.00	20.46	AAAA
ATOM	1164	CG1	VAL	A	149	40.578	24.607	54.085	1.00	19.36	AAAA
ATOM	1165	CG2	VAL	A	149	38.608	24.229	52.593	1.00	20.03	AAAA
ATOM	1166	C	VAL	A	149	39.164	23.848	56.367	1.00	21.48	AAAA
ATOM	1167	O	VAL	A	149	40.147	23.197	56.735	1.00	22.11	AAAA
ATOM	1168	N	GLU	A	150	38.628	24.826	57.088	1.00	21.19	AAAA
ATOM	1169	CA	GLU	A	150	39.171	25.176	58.386	1.00	21.70	AAAA
ATOM	1170	C	GLU	A	150	38.973	24.043	59.368	1.00	22.31	AAAA
ATOM	1171	O	GLY	A	150	39.913	23.597	60.026	1.00	22.51	AAAA
ATOM	1172	N	ILE	A	151	37.736	23.566	59.453	1.00	22.86	AAAA
ATOM	1173	CA	ILE	A	151	37.388	22.474	60.346	1.00	22.26	AAAA
ATOM	1174	CB	ILE	A	151	35.894	22.124	60.191	1.00	21.51	AAAA
ATOM	1175	CG2	ILE	A	151	35.542	20.899	61.019	1.00	21.36	AAAA
ATOM	1176	CG1	ILE	A	151	35.051	23.329	60.627	1.00	20.39	AAAA
ATOM	1177	CD1	ILE	A	151	33.576	23.199	60.361	1.00	16.88	AAAA
ATOM	1178	C	ILE	A	151	38.265	21.243	60.096	1.00	23.29	AAAA
ATOM	1179	O	ILE	A	151	38.786	20.660	61.038	1.00	23.88	AAAA
ATOM	1180	N	GLU	A	152	38.435	20.853	58.836	1.00	24.13	AAAA
ATOM	1181	CA	GLU	A	152	39.267	19.697	58.517	1.00	25.01	AAAA
ATOM	1182	CB	GLU	A	152	39.242	19.404	57.010	1.00	25.07	AAAA
ATOM	1183	CG	GLU	A	152	37.910	18.886	56.526	1.00	24.56	AAAA
ATOM	1184	CD	GLU	A	152	37.500	17.570	57.198	1.00	25.00	AAAA
ATOM	1185	OE1	GLU	A	152	36.345	17.158	57.011	1.00	26.40	AAAA
ATOM	1186	OE2	GLU	A	152	38.315	16.935	57.897	1.00	25.00	AAAA
ATOM	1187	C	GLU	A	152	40.694	19.957	58.965	1.00	26.06	AAAA
ATOM	1188	O	GLU	A	152	41.425	19.035	59.331	1.00	26.40	AAAA

Figure 19-19

ATOM	1189	N	TYR	A	153	41.085	21.225	58.925	1.00	27.30	AAAA
ATOM	1190	CA	TYR	A	153	42.422	21.632	59.334	1.00	27.63	AAAA
ATOM	1191	CB	TYR	A	153	42.532	23.153	59.268	1.00	26.99	AAAA
ATOM	1192	CG	TYR	A	153	43.856	23.719	59.710	1.00	27.03	AAAA
ATOM	1193	CD1	TYR	A	153	44.942	23.790	58.837	1.00	27.78	AAAA
ATOM	1194	CE1	TYR	A	153	46.165	24.356	59.250	1.00	28.40	AAAA
ATOM	1195	CD2	TYR	A	153	44.017	24.215	61.007	1.00	27.52	AAAA
ATOM	1196	CE2	TYR	A	153	45.216	24.774	61.425	1.00	27.66	AAAA
ATOM	1197	CZ	TYR	A	153	46.284	24.845	60.547	1.00	28.15	AAAA
ATOM	1198	OH	TYR	A	153	47.457	25.407	60.974	1.00	28.83	AAAA
ATOM	1199	C	TYR	A	153	42.618	21.172	60.769	1.00	27.82	AAAA
ATOM	1200	O	TYR	A	153	43.613	20.552	61.110	1.00	27.15	AAAA
ATOM	1201	N	LEU	A	154	41.636	21.487	61.604	1.00	29.25	AAAA
ATOM	1202	CA	LEU	A	154	41.665	21.138	63.014	1.00	29.35	AAAA
ATOM	1203	CB	LEU	A	154	40.507	21.829	63.715	1.00	30.25	AAAA
ATOM	1204	CG	LEU	A	154	40.685	23.346	63.792	1.00	31.10	AAAA
ATOM	1205	CD1	LEU	A	154	39.348	24.020	64.092	1.00	31.24	AAAA
ATOM	1206	CD2	LEU	A	154	41.747	23.669	64.852	1.00	29.84	AAAA
ATOM	1207	C	LEU	A	154	41.625	19.639	63.263	1.00	29.73	AAAA
ATOM	1208	O	LEU	A	154	42.313	19.151	64.150	1.00	30.51	AAAA
ATOM	1209	N	ARG	A	155	40.832	18.903	62.489	1.00	28.95	AAAA
ATOM	1210	CA	ARG	A	155	40.771	17.459	62.671	1.00	28.94	AAAA
ATOM	1211	CB	ARG	A	155	39.742	16.820	61.723	1.00	28.64	AAAA
ATOM	1212	CG	ARG	A	155	38.312	17.312	61.952	1.00	27.82	AAAA
ATOM	1213	CD	ARG	A	155	37.319	16.751	60.955	1.00	27.19	AAAA
ATOM	1214	NE	ARG	A	155	36.804	15.444	61.338	1.00	28.86	AAAA
ATOM	1215	CZ	ARG	A	155	35.939	14.742	60.612	1.00	28.93	AAAA
ATOM	1216	NH1	ARG	A	155	35.500	15.227	59.459	1.00	29.47	AAAA
ATOM	1217	NH2	ARG	A	155	35.486	13.574	61.053	1.00	28.76	AAAA
ATOM	1218	C	ARG	A	155	42.158	16.853	62.438	1.00	30.20	AAAA
ATOM	1219	O	ARG	A	155	42.572	15.949	63.164	1.00	30.74	AAAA
ATOM	1220	N	LYS	A	156	42.890	17.362	61.447	1.00	30.32	AAAA
ATOM	1221	CA	LYS	A	156	44.224	16.838	61.173	1.00	30.07	AAAA
ATOM	1222	CB	LYS	A	156	44.771	17.373	59.847	1.00	30.26	AAAA
ATOM	1223	CG	LYS	A	156	46.168	16.869	59.525	1.00	30.16	AAAA
ATOM	1224	CD	LYS	A	156	46.686	17.368	58.181	1.00	31.19	AAAA
ATOM	1225	CE	LYS	A	156	45.884	16.813	56.986	1.00	31.70	AAAA
ATOM	1226	NZ	LYS	A	156	45.963	15.324	56.824	1.00	31.20	AAAA
ATOM	1227	C	LYS	A	156	45.167	17.202	62.306	1.00	30.08	AAAA
ATOM	1228	O	LYS	A	156	46.192	16.550	62.485	1.00	29.16	AAAA
ATOM	1229	N	LYS	A	157	44.816	18.252	63.053	1.00	30.08	AAAA
ATOM	1230	CA	LYS	A	157	45.608	18.691	64.196	1.00	31.03	AAAA
ATOM	1231	CB	LYS	A	157	45.446	20.201	64.452	1.00	31.81	AAAA
ATOM	1232	CG	LYS	A	157	46.067	21.134	63.419	1.00	32.12	AAAA
ATOM	1233	CD	LYS	A	157	47.580	21.041	63.348	1.00	31.34	AAAA
ATOM	1234	CE	LYS	A	157	48.080	21.941	62.226	1.00	32.66	AAAA
ATOM	1235	NZ	LYS	A	157	49.556	21.921	61.996	1.00	32.74	AAAA
ATOM	1236	C	LYS	A	157	45.196	17.923	65.458	1.00	31.73	AAAA
ATOM	1237	O	LYS	A	157	45.652	18.230	66.558	1.00	31.93	AAAA
ATOM	1238	N	GLY	A	158	44.312	16.942	65.299	1.00	32.41	AAAA
ATOM	1239	CA	GLY	A	158	43.901	16.140	66.436	1.00	32.34	AAAA
ATOM	1240	C	GLY	A	158	42.604	16.429	67.172	1.00	32.65	AAAA
ATOM	1241	O	GLY	A	158	42.182	15.604	67.980	1.00	32.85	AAAA
ATOM	1242	N	PHE	A	159	41.960	17.565	66.932	1.00	33.16	AAAA
ATOM	1243	CA	PHE	A	159	40.712	17.842	67.650	1.00	34.16	AAAA
ATOM	1244	CB	PHE	A	159	40.220	19.281	67.403	1.00	34.81	AAAA
ATOM	1245	CG	PHE	A	159	41.134	20.343	67.965	1.00	34.01	AAAA
ATOM	1246	CD1	PHE	A	159	42.327	20.669	67.329	1.00	34.18	AAAA
ATOM	1247	CD2	PHE	A	159	40.821	20.981	69.166	1.00	34.61	AAAA
ATOM	1248	CE1	PHE	A	159	43.197	21.610	67.874	1.00	33.65	AAAA
ATOM	1249	CE2	PHE	A	159	41.689	21.924	69.718	1.00	34.52	AAAA
ATOM	1250	CZ	PHE	A	159	42.878	22.236	69.065	1.00	33.90	AAAA
ATOM	1251	C	PHE	A	159	39.645	16.840	67.239	1.00	34.04	AAAA
ATOM	1252	O	PHE	A	159	39.568	16.456	66.068	1.00	34.98	AAAA
ATOM	1253	N	LYS	A	160	38.839	16.403	68.202	1.00	33.36	AAAA
ATOM	1254	CA	LYS	A	160	37.794	15.415	67.936	1.00	33.11	AAAA

235/263

Figure 19-20

ATOM	1255	CB	LYS	A	160	38.060	14.140	68.763	1.00	33.97	AAAA
ATOM	1256	CG	LYS	A	160	39.410	13.491	68.457	1.00	35.31	AAAA
ATOM	1257	CD	LYS	A	160	39.833	12.364	69.429	1.00	36.48	AAAA
ATOM	1258	CE	LYS	A	160	39.095	11.037	69.243	1.00	37.97	AAAA
ATOM	1259	NZ	LYS	A	160	37.636	11.080	69.568	1.00	39.67	AAAA
ATOM	1260	C	LYS	A	160	36.385	15.941	68.210	1.00	31.68	AAAA
ATOM	1261	O	LYS	A	160	35.405	15.290	67.887	1.00	31.51	AAAA
ATOM	1262	N	ARG	A	161	36.291	17.114	68.819	1.00	31.11	AAAA
ATOM	1263	CA	ARG	A	161	35.003	17.719	69.114	1.00	30.92	AAAA
ATOM	1264	CB	ARG	A	161	34.655	17.592	70.604	1.00	31.78	AAAA
ATOM	1265	CG	ARG	A	161	34.451	16.157	71.102	1.00	32.91	AAAA
ATOM	1266	CD	ARG	A	161	33.994	16.126	72.570	1.00	33.26	AAAA
ATOM	1267	NE	ARG	A	161	34.929	16.797	73.476	1.00	34.01	AAAA
ATOM	1268	CZ	ARG	A	161	36.183	16.404	73.698	1.00	34.88	AAAA
ATOM	1269	NH1	ARG	A	161	36.675	15.334	73.081	1.00	34.89	AAAA
ATOM	1270	NH2	ARG	A	161	36.954	17.084	74.537	1.00	34.71	AAAA
ATOM	1271	C	ARG	A	161	35.061	19.185	68.714	1.00	30.28	AAAA
ATOM	1272	O	ARG	A	161	35.365	20.059	69.529	1.00	29.86	AAAA
ATOM	1273	N	ILE	A	162	34.774	19.433	67.437	1.00	28.86	AAAA
ATOM	1274	CA	ILE	A	162	34.788	20.774	66.862	1.00	26.41	AAAA
ATOM	1275	CB	ILE	A	162	35.443	20.762	65.464	1.00	26.87	AAAA
ATOM	1276	CG2	ILE	A	162	35.453	22.160	64.872	1.00	26.91	AAAA
ATOM	1277	CG1	ILE	A	162	36.877	20.234	65.578	1.00	28.19	AAAA
ATOM	1278	CD1	ILE	A	162	37.614	20.090	64.240	1.00	28.24	AAAA
ATOM	1279	C	ILE	A	162	33.369	21.283	66.731	1.00	24.08	AAAA
ATOM	1280	O	ILE	A	162	32.485	20.572	66.267	1.00	24.40	AAAA
ATOM	1281	N	LEU	A	163	33.153	22.519	67.153	1.00	22.25	AAAA
ATOM	1282	CA	LEU	A	163	31.838	23.126	67.074	1.00	20.48	AAAA
ATOM	1283	CB	LEU	A	163	31.408	23.671	68.440	1.00	20.97	AAAA
ATOM	1284	CG	LEU	A	163	30.099	24.477	68.486	1.00	20.50	AAAA
ATOM	1285	CD1	LEU	A	163	28.998	23.695	67.799	1.00	19.07	AAAA
ATOM	1286	CD2	LEU	A	163	29.738	24.802	69.950	1.00	19.76	AAAA
ATOM	1287	C	LEU	A	163	31.801	24.241	66.055	1.00	18.76	AAAA
ATOM	1288	O	LEU	A	163	32.756	24.986	65.894	1.00	18.41	AAAA
ATOM	1289	N	TYR	A	164	30.677	24.344	65.368	1.00	17.85	AAAA
ATOM	1290	CA	TYR	A	164	30.496	25.372	64.373	1.00	17.16	AAAA
ATOM	1291	CB	TYR	A	164	30.644	24.768	62.983	1.00	17.45	AAAA
ATOM	1292	CG	TYR	A	164	30.484	25.783	61.900	1.00	17.70	AAAA
ATOM	1293	CD1	TYR	A	164	31.444	26.772	61.701	1.00	16.23	AAAA
ATOM	1294	CE1	TYR	A	164	31.280	27.734	60.721	1.00	17.35	AAAA
ATOM	1295	CD2	TYR	A	164	29.350	25.781	61.092	1.00	17.95	AAAA
ATOM	1296	CE2	TYR	A	164	29.173	26.746	60.103	1.00	18.03	AAAA
ATOM	1297	CZ	TYR	A	164	30.138	27.717	59.919	1.00	17.30	AAAA
ATOM	1298	OH	TYR	A	164	29.955	28.647	58.926	1.00	16.70	AAAA
ATOM	1299	C	TYR	A	164	29.123	26.016	64.514	1.00	15.85	AAAA
ATOM	1300	O	TYR	A	164	28.101	25.351	64.416	1.00	16.44	AAAA
ATOM	1301	N	ILE	A	165	29.115	27.319	64.743	1.00	15.54	AAAA
ATOM	1302	CA	ILE	A	165	27.878	28.088	64.897	1.00	15.71	AAAA
ATOM	1303	CB	ILE	A	165	27.869	28.819	66.250	1.00	15.18	AAAA
ATOM	1304	CG2	ILE	A	165	26.621	29.685	66.374	1.00	13.94	AAAA
ATOM	1305	CG1	ILE	A	165	28.000	27.797	67.386	1.00	13.94	AAAA
ATOM	1306	CD1	ILE	A	165	28.356	28.421	68.747	1.00	13.94	AAAA
ATOM	1307	C	ILE	A	165	27.808	29.124	63.754	1.00	16.00	AAAA
ATOM	1308	O	ILE	A	165	28.711	29.941	63.576	1.00	16.56	AAAA
ATOM	1309	N	ASP	A	166	26.721	29.087	63.001	1.00	16.18	AAAA
ATOM	1310	CA	ASP	A	166	26.524	29.962	61.865	1.00	16.67	AAAA
ATOM	1311	CB	ASP	A	166	26.240	29.066	60.651	1.00	18.05	AAAA
ATOM	1312	CG	ASP	A	166	26.238	29.809	59.329	1.00	19.21	AAAA
ATOM	1313	OD1	ASP	A	166	25.353	30.659	59.114	1.00	18.36	AAAA
ATOM	1314	OD2	ASP	A	166	27.131	29.521	58.495	1.00	19.19	AAAA
ATOM	1315	C	ASP	A	166	25.342	30.904	62.169	1.00	17.57	AAAA
ATOM	1316	O	ASP	A	166	24.206	30.459	62.321	1.00	17.26	AAAA
ATOM	1317	N	LEU	A	167	25.605	32.202	62.274	1.00	16.67	AAAA
ATOM	1318	CA	LEU	A	167	24.526	33.135	62.562	1.00	16.89	AAAA
ATOM	1319	CB	LEU	A	167	24.923	34.116	63.663	1.00	17.27	AAAA
ATOM	1320	CG	LEU	A	167	25.499	33.529	64.954	1.00	18.37	AAAA

Figure 19-21

ATOM	1321	CD1	LEU	A	167	25.760	34.671	65.933	1.00	18.72	AAAA
ATOM	1322	CD2	LEU	A	167	24.566	32.507	65.547	1.00	17.06	AAAA
ATOM	1323	C	LEU	A	167	24.146	33.897	61.307	1.00	17.18	AAAA
ATOM	1324	O	LEU	A	167	23.390	34.850	61.358	1.00	17.21	AAAA
ATOM	1325	N	ASP	A	168	24.683	33.457	60.178	1.00	17.83	AAAA
ATOM	1326	CA	ASP	A	168	24.382	34.067	58.904	1.00	17.84	AAAA
ATOM	1327	CB	ASP	A	168	25.178	33.397	57.807	1.00	20.42	AAAA
ATOM	1328	CG	ASP	A	168	25.140	34.162	56.529	1.00	21.41	AAAA
ATOM	1329	C	ASP	A	168	22.915	33.783	58.660	1.00	18.35	AAAA
ATOM	1330	O	ASP	A	168	22.419	32.722	59.032	1.00	19.62	AAAA
ATOM	1331	OD1	ASP	A	168	26.066	34.972	56.330	1.00	22.42	AAAA
ATOM	1332	OD2	ASP	A	168	24.186	33.971	55.746	1.00	21.79	AAAA
ATOM	1333	N	ALA	A	169	22.239	34.717	58.010	1.00	17.98	AAAA
ATOM	1334	CA	ALA	A	169	20.824	34.601	57.708	1.00	17.36	AAAA
ATOM	1335	CB	ALA	A	169	20.348	35.860	57.007	1.00	17.00	AAAA
ATOM	1336	C	ALA	A	169	20.439	33.377	56.887	1.00	18.64	AAAA
ATOM	1337	O	ALA	A	169	19.255	33.043	56.819	1.00	19.46	AAAA
ATOM	1338	N	HIS	A	170	21.412	32.712	56.262	1.00	18.71	AAAA
ATOM	1339	CA	HIS	A	170	21.107	31.518	55.464	1.00	18.43	AAAA
ATOM	1340	C	HIS	A	170	21.802	30.265	55.986	1.00	18.02	AAAA
ATOM	1341	O	HIS	A	170	22.910	30.332	56.514	1.00	17.20	AAAA
ATOM	1342	CB	HIS	A	170	21.539	31.678	54.004	1.00	18.79	AAAA
ATOM	1343	CG	HIS	A	170	21.137	32.968	53.386	1.00	17.65	AAAA
ATOM	1344	ND1	HIS	A	170	21.644	34.162	53.828	1.00	18.08	AAAA
ATOM	1345	CE1	HIS	A	170	21.112	35.081	53.054	1.00	18.95	AAAA
ATOM	1346	CD2	HIS	A	170	20.301	33.194	52.348	1.00	18.81	AAAA
ATOM	1347	NE2	HIS	A	170	20.291	34.544	52.140	1.00	19.66	AAAA
ATOM	1348	N	HIS	A	171	21.142	29.124	55.793	1.00	17.53	AAAA
ATOM	1349	CA	HIS	A	171	21.662	27.822	56.193	1.00	16.38	AAAA
ATOM	1350	CB	HIS	A	171	20.644	26.740	55.830	1.00	16.32	AAAA
ATOM	1351	CG	HIS	A	171	21.157	25.337	55.958	1.00	15.91	AAAA
ATOM	1352	CD2	HIS	A	171	21.241	24.336	55.051	1.00	14.14	AAAA
ATOM	1353	ND1	HIS	A	171	21.602	24.807	57.151	1.00	16.79	AAAA
ATOM	1354	CE1	HIS	A	171	21.937	23.543	56.973	1.00	14.91	AAAA
ATOM	1355	NE2	HIS	A	171	21.725	23.234	55.709	1.00	15.45	AAAA
ATOM	1356	C	HIS	A	171	22.982	27.522	55.509	1.00	16.94	AAAA
ATOM	1357	O	HIS	A	171	23.146	27.725	54.318	1.00	18.71	AAAA
ATOM	1358	N	CYS	A	172	23.926	27.019	56.279	1.00	16.99	AAAA
ATOM	1359	CA	CYS	A	172	25.237	26.670	55.778	1.00	16.23	AAAA
ATOM	1360	CB	CYS	A	172	26.219	26.721	56.947	1.00	17.89	AAAA
ATOM	1361	SG	CYS	A	172	25.638	25.773	58.397	1.00	17.89	AAAA
ATOM	1362	C	CYS	A	172	25.205	25.271	55.210	1.00	16.57	AAAA
ATOM	1363	O	CYS	A	172	25.947	24.413	55.670	1.00	17.66	AAAA
ATOM	1364	N	ASP	A	173	24.364	25.026	54.214	1.00	18.25	AAAA
ATOM	1365	CA	ASP	A	173	24.253	23.680	53.620	1.00	19.91	AAAA
ATOM	1366	CB	ASP	A	173	23.342	23.699	52.397	1.00	20.86	AAAA
ATOM	1367	CG	ASP	A	173	23.780	24.719	51.358	1.00	21.90	AAAA
ATOM	1368	OD1	ASP	A	173	23.257	24.640	50.217	1.00	21.35	AAAA
ATOM	1369	OD2	ASP	A	173	24.624	25.597	51.687	1.00	21.35	AAAA
ATOM	1370	C	ASP	A	173	25.573	23.021	53.227	1.00	21.02	AAAA
ATOM	1371	O	ASP	A	173	25.673	21.785	53.199	1.00	22.79	AAAA
ATOM	1372	N	GLY	A	174	26.579	23.832	52.912	1.00	20.03	AAAA
ATOM	1373	CA	GLY	A	174	27.870	23.277	52.553	1.00	19.72	AAAA
ATOM	1374	C	GLY	A	174	28.537	22.680	53.771	1.00	20.27	AAAA
ATOM	1375	O	GLY	A	174	29.110	21.599	53.711	1.00	19.77	AAAA
ATOM	1376	N	VAL	A	175	28.448	23.387	54.893	1.00	21.38	AAAA
ATOM	1377	CA	VAL	A	175	29.056	22.934	56.135	1.00	22.26	AAAA
ATOM	1378	CB	VAL	A	175	29.032	24.040	57.203	1.00	23.15	AAAA
ATOM	1379	CG1	VAL	A	175	29.853	23.617	58.418	1.00	22.84	AAAA
ATOM	1380	CG2	VAL	A	175	29.562	25.347	56.612	1.00	23.43	AAAA
ATOM	1381	C	VAL	A	175	28.302	21.724	56.654	1.00	23.51	AAAA
ATOM	1382	O	VAL	A	175	28.893	20.803	57.210	1.00	23.74	AAAA
ATOM	1383	N	GLN	A	176	26.993	21.721	56.452	1.00	24.80	AAAA
ATOM	1384	CA	GLN	A	176	26.171	20.601	56.893	1.00	25.41	AAAA
ATOM	1385	CB	GLN	A	176	24.689	20.913	56.694	1.00	24.77	AAAA
ATOM	1386	CG	GLN	A	176	23.799	19.735	57.036	1.00	26.23	AAAA

237/263

Figure 19-22

ATOM	1387	CD	GLN	A	176	22.334	20.094	57.069	1.00	27.17	AAAA
ATOM	1388	OE1	GLN	A	176	21.902	20.879	57.911	1.00	28.24	AAAA
ATOM	1389	NE2	GLN	A	176	21.556	19.522	56.151	1.00	26.54	AAAA
ATOM	1390	C	GLN	A	176	26.512	19.293	56.180	1.00	25.67	AAAA
ATOM	1391	O	GLN	A	176	26.789	18.285	56.820	1.00	26.98	AAAA
ATOM	1392	N	GLU	A	177	26.490	19.309	54.853	1.00	26.34	AAAA
ATOM	1393	CA	GLU	A	177	26.786	18.117	54.073	1.00	26.18	AAAA
ATOM	1394	CB	GLU	A	177	26.746	18.468	52.580	1.00	27.13	AAAA
ATOM	1395	CG	GLU	A	177	26.769	17.269	51.628	1.00	29.77	AAAA
ATOM	1396	CD	GLU	A	177	26.623	17.660	50.147	1.00	31.29	AAAA
ATOM	1397	OE1	GLU	A	177	27.655	17.935	49.500	1.00	31.35	AAAA
ATOM	1398	OE2	GLU	A	177	25.471	17.703	49.636	1.00	32.05	AAAA
ATOM	1399	C	GLU	A	177	28.160	17.556	54.460	1.00	26.38	AAAA
ATOM	1400	O	GLU	A	177	28.338	16.349	54.595	1.00	25.41	AAAA
ATOM	1401	N	ALA	A	178	29.115	18.458	54.659	1.00	27.58	AAAA
ATOM	1402	CA	ALA	A	178	30.495	18.119	55.004	1.00	27.66	AAAA
ATOM	1403	CB	ALA	A	178	31.345	19.385	54.994	1.00	26.20	AAAA
ATOM	1404	C	ALA	A	178	30.713	17.370	56.318	1.00	28.33	AAAA
ATOM	1405	O	ALA	A	178	31.685	16.626	56.439	1.00	29.44	AAAA
ATOM	1406	N	PHE	A	179	29.849	17.564	57.308	1.00	28.25	AAAA
ATOM	1407	CA	PHE	A	179	30.036	16.852	58.561	1.00	29.20	AAAA
ATOM	1408	CB	PHE	A	179	30.570	17.794	59.624	1.00	29.35	AAAA
ATOM	1409	CG	PHE	A	179	31.751	18.572	59.171	1.00	30.26	AAAA
ATOM	1410	CD1	PHE	A	179	31.582	19.777	58.497	1.00	31.01	AAAA
ATOM	1411	CD2	PHE	A	179	33.033	18.069	59.339	1.00	30.37	AAAA
ATOM	1412	CE1	PHE	A	179	32.670	20.470	57.993	1.00	31.20	AAAA
ATOM	1413	CE2	PHE	A	179	34.133	18.749	58.840	1.00	31.74	AAAA
ATOM	1414	CZ	PHE	A	179	33.950	19.960	58.161	1.00	31.81	AAAA
ATOM	1415	C	PHE	A	179	28.760	16.180	59.040	1.00	30.33	AAAA
ATOM	1416	O	PHE	A	179	28.624	15.810	60.215	1.00	31.82	AAAA
ATOM	1417	N	TYR	A	180	27.842	15.994	58.105	1.00	29.18	AAAA
ATOM	1418	CA	TYR	A	180	26.564	15.379	58.389	1.00	28.99	AAAA
ATOM	1419	CB	TYR	A	180	25.725	15.343	57.123	1.00	28.30	AAAA
ATOM	1420	CG	TYR	A	180	24.244	15.422	57.384	1.00	28.27	AAAA
ATOM	1421	CD1	TYR	A	180	23.392	14.386	57.021	1.00	27.05	AAAA
ATOM	1422	CE1	TYR	A	180	22.029	14.491	57.197	1.00	28.51	AAAA
ATOM	1423	CD2	TYR	A	180	23.686	16.573	57.942	1.00	29.34	AAAA
ATOM	1424	CE2	TYR	A	180	22.316	16.691	58.125	1.00	29.27	AAAA
ATOM	1425	CZ	TYR	A	180	21.495	15.645	57.746	1.00	29.33	AAAA
ATOM	1426	OH	TYR	A	180	20.141	15.775	57.893	1.00	30.83	AAAA
ATOM	1427	C	TYR	A	180	26.673	13.970	58.940	1.00	28.79	AAAA
ATOM	1428	O	TYR	A	180	25.877	13.577	59.785	1.00	28.71	AAAA
ATOM	1429	N	ASP	A	181	27.662	13.214	58.472	1.00	29.03	AAAA
ATOM	1430	CA	ASP	A	181	27.813	11.828	58.914	1.00	28.49	AAAA
ATOM	1431	CB	ASP	A	181	28.140	10.930	57.715	1.00	27.59	AAAA
ATOM	1432	CG	ASP	A	181	29.548	11.122	57.229	1.00	28.82	AAAA
ATOM	1433	OD1	ASP	A	181	29.981	12.292	57.183	1.00	29.25	AAAA
ATOM	1434	OD2	ASP	A	181	30.216	10.119	56.887	1.00	28.68	AAAA
ATOM	1435	C	ASP	A	181	28.863	11.631	60.009	1.00	27.67	AAAA
ATOM	1436	O	ASP	A	181	29.271	10.504	60.293	1.00	27.57	AAAA
ATOM	1437	N	THR	A	182	29.308	12.713	60.628	1.00	26.27	AAAA
ATOM	1438	CA	THR	A	182	30.284	12.544	61.689	1.00	26.22	AAAA
ATOM	1439	CB	THR	A	182	31.670	13.118	61.317	1.00	25.92	AAAA
ATOM	1440	OG1	THR	A	182	32.564	12.935	62.416	1.00	25.06	AAAA
ATOM	1441	CG2	THR	A	182	31.577	14.594	60.974	1.00	25.25	AAAA
ATOM	1442	C	THR	A	182	29.792	13.223	62.934	1.00	25.87	AAAA
ATOM	1443	O	THR	A	182	28.942	14.102	62.863	1.00	26.35	AAAA
ATOM	1444	N	ASP	A	183	30.327	12.804	64.071	1.00	25.86	AAAA
ATOM	1445	CA	ASP	A	183	29.953	13.370	65.355	1.00	26.12	AAAA
ATOM	1446	CB	ASP	A	183	29.468	12.260	66.274	1.00	27.10	AAAA
ATOM	1447	CG	ASP	A	183	30.515	11.194	66.488	1.00	28.80	AAAA
ATOM	1448	OD1	ASP	A	183	31.063	10.691	65.480	1.00	29.78	AAAA
ATOM	1449	OD2	ASP	A	183	30.781	10.852	67.657	1.00	29.21	AAAA
ATOM	1450	C	ASP	A	183	31.126	14.120	65.995	1.00	26.77	AAAA
ATOM	1451	O	ASP	A	183	31.034	14.566	67.146	1.00	26.65	AAAA
ATOM	1452	N	GLN	A	184	32.229	14.254	65.254	1.00	26.05	AAAA

238/263 Figure 19-23

ATOM	1453	CA	GLN	A	184	33.381	14.983	65.766	1.00	25.85	AAAA
ATOM	1454	CB	GLN	A	184	34.674	14.510	65.095	1.00	26.30	AAAA
ATOM	1455	CG	GLN	A	184	34.920	13.030	65.303	1.00	27.42	AAAA
ATOM	1456	CD	GLN	A	184	36.273	12.583	64.822	1.00	28.40	AAAA
ATOM	1457	OE1	GLN	A	184	36.685	12.905	63.709	1.00	30.05	AAAA
ATOM	1458	NE2	GLN	A	184	36.970	11.816	65.651	1.00	29.24	AAAA
ATOM	1459	C	GLN	A	184	33.159	16.474	65.536	1.00	25.22	AAAA
ATOM	1460	O	GLN	A	184	33.734	17.316	66.220	1.00	24.57	AAAA
ATOM	1461	N	VAL	A	185	32.290	16.791	64.584	1.00	25.17	AAAA
ATOM	1462	CA	VAL	A	185	31.975	18.182	64.291	1.00	24.49	AAAA
ATOM	1463	CB	VAL	A	185	32.324	18.563	62.832	1.00	23.20	AAAA
ATOM	1464	CG1	VAL	A	185	32.045	20.060	62.599	1.00	19.72	AAAA
ATOM	1465	CG2	VAL	A	185	33.777	18.205	62.543	1.00	20.67	AAAA
ATOM	1466	C	VAL	A	185	30.494	18.421	64.501	1.00	24.81	AAAA
ATOM	1467	O	VAL	A	185	29.664	17.787	63.844	1.00	27.07	AAAA
ATOM	1468	N	PHE	A	186	30.162	19.311	65.434	1.00	23.40	AAAA
ATOM	1469	CA	PHE	A	186	28.768	19.645	65.684	1.00	20.31	AAAA
ATOM	1470	CB	PHE	A	186	28.513	19.937	67.164	1.00	19.77	AAAA
ATOM	1471	CG	PHE	A	186	27.057	20.037	67.500	1.00	18.55	AAAA
ATOM	1472	CD1	PHE	A	186	26.359	18.918	67.945	1.00	17.70	AAAA
ATOM	1473	CD2	PHE	A	186	26.358	21.213	67.263	1.00	17.46	AAAA
ATOM	1474	CE1	PHE	A	186	24.999	18.964	68.147	1.00	17.35	AAAA
ATOM	1475	CE2	PHE	A	186	24.997	21.271	67.459	1.00	18.83	AAAA
ATOM	1476	CZ	PHE	A	186	24.308	20.138	67.905	1.00	18.67	AAAA
ATOM	1477	C	PHE	A	186	28.464	20.911	64.895	1.00	19.18	AAAA
ATOM	1478	O	PHE	A	186	29.079	21.940	65.129	1.00	18.82	AAAA
ATOM	1479	N	VAL	A	187	27.520	20.834	63.964	1.00	18.34	AAAA
ATOM	1480	CA	VAL	A	187	27.137	21.993	63.160	1.00	16.47	AAAA
ATOM	1481	CB	VAL	A	187	27.006	21.630	61.655	1.00	14.30	AAAA
ATOM	1482	CG1	VAL	A	187	26.628	22.869	60.828	1.00	10.34	AAAA
ATOM	1483	CG2	VAL	A	187	28.314	21.031	61.160	1.00	12.07	AAAA
ATOM	1484	C	VAL	A	187	25.806	22.511	63.665	1.00	17.43	AAAA
ATOM	1485	O	VAL	A	187	24.852	21.746	63.792	1.00	16.95	AAAA
ATOM	1486	N	LEU	A	188	25.763	23.809	63.960	1.00	18.66	AAAA
ATOM	1487	CA	LEU	A	188	24.555	24.507	64.460	1.00	20.51	AAAA
ATOM	1488	CB	LEU	A	188	24.752	24.995	65.914	1.00	21.24	AAAA
ATOM	1489	CG	LEU	A	188	23.702	26.019	66.395	1.00	20.80	AAAA
ATOM	1490	CD1	LEU	A	188	22.365	25.323	66.493	1.00	19.77	AAAA
ATOM	1491	CD2	LEU	A	188	24.085	26.627	67.750	1.00	20.63	AAAA
ATOM	1492	C	LEU	A	188	24.297	25.735	63.591	1.00	20.41	AAAA
ATOM	1493	O	LEU	A	188	25.223	26.484	63.288	1.00	21.86	AAAA
ATOM	1494	N	SER	A	189	23.049	25.987	63.233	1.00	19.32	AAAA
ATOM	1495	CA	SER	A	189	22.786	27.130	62.381	1.00	18.06	AAAA
ATOM	1496	CB	SER	A	189	22.970	26.715	60.906	1.00	18.54	AAAA
ATOM	1497	OG	SER	A	189	22.559	27.731	59.998	1.00	17.47	AAAA
ATOM	1498	C	SER	A	189	21.418	27.751	62.554	1.00	17.90	AAAA
ATOM	1499	O	SER	A	189	20.404	27.051	62.540	1.00	19.54	AAAA
ATOM	1500	N	LEU	A	190	21.386	29.067	62.722	1.00	16.97	AAAA
ATOM	1501	CA	LEU	A	190	20.117	29.772	62.797	1.00	18.49	AAAA
ATOM	1502	CB	LEU	A	190	20.097	30.865	63.886	1.00	17.78	AAAA
ATOM	1503	CG	LEU	A	190	20.534	30.600	65.337	1.00	17.10	AAAA
ATOM	1504	CD1	LEU	A	190	19.643	31.406	66.266	1.00	15.50	AAAA
ATOM	1505	CD2	LEU	A	190	20.455	29.147	65.686	1.00	15.15	AAAA
ATOM	1506	C	LEU	A	190	20.111	30.408	61.416	1.00	19.35	AAAA
ATOM	1507	O	LEU	A	190	21.136	30.891	60.967	1.00	19.75	AAAA
ATOM	1508	N	HIS	A	191	18.975	30.397	60.736	1.00	21.75	AAAA
ATOM	1509	CA	HIS	A	191	18.897	30.955	59.383	1.00	23.55	AAAA
ATOM	1510	CB	HIS	A	191	19.626	30.013	58.426	1.00	23.63	AAAA
ATOM	1511	CG	HIS	A	191	19.157	28.597	58.533	1.00	24.26	AAAA
ATOM	1512	CD2	HIS	A	191	19.770	27.485	59.009	1.00	23.78	AAAA
ATOM	1513	ND1	HIS	A	191	17.869	28.217	58.217	1.00	24.73	AAAA
ATOM	1514	CE1	HIS	A	191	17.709	26.935	58.491	1.00	23.90	AAAA
ATOM	1515	NE2	HIS	A	191	18.849	26.467	58.973	1.00	24.51	AAAA
ATOM	1516	C	HIS	A	191	17.446	31.119	58.926	1.00	24.10	AAAA
ATOM	1517	O	HIS	A	191	16.519	30.658	59.596	1.00	24.94	AAAA
ATOM	1518	N	GLN	A	192	17.249	31.789	57.794	1.00	24.33	AAAA

239/263

Figure 19-24

ATOM	1519	CA	GLN	A	192	15.899	31.959	57.269	1.00	25.77	AAAA
ATOM	1520	CB	GLN	A	192	15.881	32.896	56.060	1.00	26.51	AAAA
ATOM	1521	CG	GLN	A	192	16.467	34.271	56.325	1.00	26.99	AAAA
ATOM	1522	CD	GLN	A	192	16.581	35.076	55.062	1.00	27.98	AAAA
ATOM	1523	OE1	GLN	A	192	15.583	35.496	54.493	1.00	30.48	AAAA
ATOM	1524	NE2	GLN	A	192	17.802	35.274	54.595	1.00	29.04	AAAA
ATOM	1525	C	GLN	A	192	15.463	30.573	56.832	1.00	25.77	AAAA
ATOM	1526	O	GLN	A	192	16.211	29.865	56.169	1.00	26.73	AAAA
ATOM	1527	N	SER	A	193	14.259	30.184	57.214	1.00	25.48	AAAA
ATOM	1528	CA	SER	A	193	13.750	28.877	56.863	1.00	24.51	AAAA
ATOM	1529	CB	SER	A	193	12.288	28.788	57.286	1.00	23.77	AAAA
ATOM	1530	OG	SER	A	193	11.753	27.517	57.010	1.00	24.81	AAAA
ATOM	1531	C	SER	A	193	13.906	28.597	55.361	1.00	24.53	AAAA
ATOM	1532	O	SER	A	193	13.736	29.479	54.522	1.00	22.32	AAAA
ATOM	1533	N	PRO	A	194	14.226	27.348	55.007	1.00	25.69	AAAA
ATOM	1534	CD	PRO	A	194	14.411	26.167	55.862	1.00	25.02	AAAA
ATOM	1535	CA	PRO	A	194	14.399	26.976	53.604	1.00	27.05	AAAA
ATOM	1536	CB	PRO	A	194	14.906	25.535	53.697	1.00	26.30	AAAA
ATOM	1537	CG	PRO	A	194	15.479	25.466	55.124	1.00	26.44	AAAA
ATOM	1538	C	PRO	A	194	13.076	27.057	52.849	1.00	27.79	AAAA
ATOM	1539	O	PRO	A	194	13.066	27.057	51.625	1.00	28.82	AAAA
ATOM	1540	N	GLU	A	195	11.966	27.133	53.582	1.00	28.29	AAAA
ATOM	1541	CA	GLU	A	195	10.656	27.187	52.950	1.00	29.08	AAAA
ATOM	1542	CB	GLU	A	195	9.534	27.030	54.001	1.00	31.08	AAAA
ATOM	1543	CG	GLU	A	195	9.070	28.294	54.722	1.00	35.07	AAAA
ATOM	1544	CD	GLU	A	195	7.850	28.980	54.064	1.00	38.05	AAAA
ATOM	1545	OE1	GLU	A	195	7.389	30.017	54.601	1.00	38.80	AAAA
ATOM	1546	OE2	GLU	A	195	7.342	28.487	53.024	1.00	39.20	AAAA
ATOM	1547	C	GLU	A	195	10.483	28.471	52.150	1.00	28.05	AAAA
ATOM	1548	O	GLU	A	195	9.722	28.512	51.189	1.00	28.57	AAAA
ATOM	1549	N	TYR	A	196	11.223	29.510	52.514	1.00	27.39	AAAA
ATOM	1550	CA	TYR	A	196	11.108	30.769	51.802	1.00	25.80	AAAA
ATOM	1551	CB	TYR	A	196	10.275	31.743	52.645	1.00	24.97	AAAA
ATOM	1552	CG	TYR	A	196	10.971	32.281	53.868	1.00	23.41	AAAA
ATOM	1553	CD1	TYR	A	196	11.911	33.306	53.765	1.00	23.99	AAAA
ATOM	1554	CE1	TYR	A	196	12.559	33.805	54.892	1.00	23.44	AAAA
ATOM	1555	CD2	TYR	A	196	10.697	31.768	55.126	1.00	23.24	AAAA
ATOM	1556	CE2	TYR	A	196	11.336	32.256	56.254	1.00	23.93	AAAA
ATOM	1557	CZ	TYR	A	196	12.265	33.270	56.133	1.00	24.07	AAAA
ATOM	1558	OH	TYR	A	196	12.913	33.731	57.247	1.00	25.06	AAAA
ATOM	1559	C	TYR	A	196	12.450	31.406	51.411	1.00	24.97	AAAA
ATOM	1560	O	TYR	A	196	12.475	32.495	50.840	1.00	25.14	AAAA
ATOM	1561	N	ALA	A	197	13.563	30.737	51.686	1.00	23.81	AAAA
ATOM	1562	CA	ALA	A	197	14.855	31.330	51.337	1.00	23.32	AAAA
ATOM	1563	CB	ALA	A	197	15.350	32.220	52.488	1.00	23.33	AAAA
ATOM	1564	C	ALA	A	197	15.952	30.356	50.957	1.00	22.74	AAAA
ATOM	1565	O	ALA	A	197	15.951	29.207	51.37	1.00	22.47	AAAA
ATOM	1566	N	PHE	A	198	16.900	30.852	50.16	1.00	23.23	AAAA
ATOM	1567	CA	PHE	A	198	18.062	30.081	49.741	1.00	23.68	AAAA
ATOM	1568	CB	PHE	A	198	19.083	31.006	49.069	1.00	23.33	AAAA
ATOM	1569	CG	PHE	A	198	20.250	30.280	48.464	1.00	22.98	AAAA
ATOM	1570	CD1	PHE	A	198	20.151	29.713	47.203	1.00	22.75	AAAA
ATOM	1571	CD2	PHE	A	198	21.436	30.127	49.175	1.00	23.32	AAAA
ATOM	1572	CE1	PHE	A	198	21.207	29.003	46.645	1.00	22.13	AAAA
ATOM	1573	CE2	PHE	A	198	22.512	29.408	48.622	1.00	22.83	AAAA
ATOM	1574	CZ	PHE	A	198	22.386	28.849	47.351	1.00	22.55	AAAA
ATOM	1575	C	PHE	A	198	18.689	29.490	51.008	1.00	23.69	AAAA
ATOM	1576	O	PHE	A	198	18.802	30.171	52.012	1.00	22.85	AAAA
ATOM	1577	N	PRO	A	199	19.166	28.236	50.954	1.00	23.96	AAAA
ATOM	1578	CD	PRO	A	199	19.833	27.639	52.123	1.00	24.26	AAAA
ATOM	1579	CA	PRO	A	199	19.199	27.286	49.837	1.00	24.70	AAAA
ATOM	1580	CB	PRO	A	199	20.163	26.222	50.357	1.00	23.30	AAAA
ATOM	1581	CG	PRO	A	199	19.797	26.162	51.782	1.00	23.21	AAAA
ATOM	1582	C	PRO	A	199	17.885	26.679	49.326	1.00	25.22	AAAA
ATOM	1583	O	PRO	A	199	17.866	26.145	48.215	1.00	26.24	AAAA
ATOM	1584	N	PHE	A	200	16.811	26.756	50.116	1.00	25.09	AAAA

Figure 19-25

ATOM	1585	CA	PHE	A	200	15.497	26.190	49.763	1.00	26.29	AAAA
ATOM	1586	CB	PHE	A	200	15.064	26.567	48.340	1.00	25.65	AAAA
ATOM	1587	CG	PHE	A	200	14.863	28.035	48.122	1.00	24.65	AAAA
ATOM	1588	CD1	PHE	A	200	15.806	28.781	47.439	1.00	24.42	AAAA
ATOM	1589	CD2	PHE	A	200	13.735	28.671	48.608	1.00	23.79	AAAA
ATOM	1590	CE1	PHE	A	200	15.631	30.125	47.246	1.00	24.41	AAAA
ATOM	1591	CE2	PHE	A	200	13.552	30.035	48.418	1.00	24.94	AAAA
ATOM	1592	CZ	PHE	A	200	14.499	30.760	47.738	1.00	24.57	AAAA
ATOM	1593	C	PHE	A	200	15.415	24.656	49.863	1.00	28.54	AAAA
ATOM	1594	O	PHE	A	200	14.386	24.096	50.251	1.00	28.76	AAAA
ATOM	1595	N	GLU	A	201	16.499	23.981	49.504	1.00	29.67	AAAA
ATOM	1596	CA	GLU	A	201	16.539	22.528	49.524	1.00	31.88	AAAA
ATOM	1597	CB	GLU	A	201	17.434	22.045	48.392	1.00	32.71	AAAA
ATOM	1598	CG	GLU	A	201	16.897	22.415	47.017	1.00	34.87	AAAA
ATOM	1599	CD	GLU	A	201	17.898	22.147	45.912	1.00	35.14	AAAA
ATOM	1600	OE1	GLU	A	201	18.299	20.982	45.735	1.00	36.09	AAAA
ATOM	1601	OE2	GLU	A	201	18.286	23.112	45.221	1.00	36.30	AAAA
ATOM	1602	C	GLU	A	201	16.997	21.894	50.835	1.00	32.77	AAAA
ATOM	1603	O	GLU	A	201	16.806	20.690	51.046	1.00	33.44	AAAA
ATOM	1604	N	LYS	A	202	17.599	22.690	51.711	1.00	32.31	AAAA
ATOM	1605	CA	LYS	A	202	18.101	22.168	52.974	1.00	32.09	AAAA
ATOM	1606	CB	LYS	A	202	19.565	21.750	52.811	1.00	33.02	AAAA
ATOM	1607	CG	LYS	A	202	19.836	20.847	51.623	1.00	34.95	AAAA
ATOM	1608	CD	LYS	A	202	21.334	20.619	51.436	1.00	37.92	AAAA
ATOM	1609	CE	LYS	A	202	21.655	19.804	50.169	1.00	39.19	AAAA
ATOM	1610	NZ	LYS	A	202	23.120	19.522	49.988	1.00	38.58	AAAA
ATOM	1611	C	LYS	A	202	17.995	23.241	54.037	1.00	30.85	AAAA
ATOM	1612	O	LYS	A	202	17.706	24.389	53.739	1.00	30.49	AAAA
ATOM	1613	N	GLY	A	203	18.238	22.867	55.281	1.00	30.81	AAAA
ATOM	1614	CA	GLY	A	203	18.159	23.831	56.356	1.00	30.86	AAAA
ATOM	1615	C	GLY	A	203	16.991	23.578	57.280	1.00	30.84	AAAA
ATOM	1616	O	GLY	A	203	16.828	24.285	58.272	1.00	31.58	AAAA
ATOM	1617	N	PHE	A	204	16.182	22.570	56.965	1.00	30.54	AAAA
ATOM	1618	CA	PHE	A	204	15.025	22.241	57.797	1.00	30.51	AAAA
ATOM	1619	CB	PHE	A	204	14.061	21.317	57.058	1.00	29.06	AAAA
ATOM	1620	CG	PHE	A	204	13.524	21.890	55.787	1.00	27.13	AAAA
ATOM	1621	CD1	PHE	A	204	14.222	21.762	54.601	1.00	26.52	AAAA
ATOM	1622	CD2	PHE	A	204	12.307	22.548	55.779	1.00	26.50	AAAA
ATOM	1623	CE1	PHE	A	204	13.713	22.276	53.420	1.00	26.44	AAAA
ATOM	1624	CE2	PHE	A	204	11.786	23.069	54.600	1.00	26.69	AAAA
ATOM	1625	CZ	PHE	A	204	12.490	22.931	53.416	1.00	25.65	AAAA
ATOM	1626	C	PHE	A	204	15.401	21.590	59.127	1.00	30.87	AAAA
ATOM	1627	O	PHE	A	204	16.395	20.875	59.228	1.00	31.12	AAAA
ATOM	1628	N	LEU	A	205	14.580	21.844	60.139	1.00	31.22	AAAA
ATOM	1629	CA	LEU	A	205	14.782	21.329	61.489	1.00	31.43	AAAA
ATOM	1630	CB	LEU	A	205	13.575	21.691	62.357	1.00	31.42	AAAA
ATOM	1631	CG	LEU	A	205	13.603	21.078	63.755	1.00	31.76	AAAA
ATOM	1632	CD1	LEU	A	205	14.894	21.492	64.457	1.00	32.36	AAAA
ATOM	1633	CD2	LEU	A	205	12.379	21.516	64.536	1.00	31.31	AAAA
ATOM	1634	C	LEU	A	205	15.026	19.829	61.625	1.00	31.35	AAAA
ATOM	1635	O	LEU	A	205	15.714	19.392	62.546	1.00	31.40	AAAA
ATOM	1636	N	GLU	A	206	14.448	19.059	60.707	1.00	31.79	AAAA
ATOM	1637	CA	GLU	A	206	14.509	17.603	60.706	1.00	32.08	AAAA
ATOM	1638	CB	GLU	A	206	13.485	17.054	59.716	1.00	33.18	AAAA
ATOM	1639	CG	GLU	A	206	12.069	17.651	59.829	1.00	34.20	AAAA
ATOM	1640	CD	GLU	A	206	11.973	19.136	59.453	1.00	33.44	AAAA
ATOM	1641	OE1	GLU	A	206	10.854	19.675	59.422	1.00	33.32	AAAA
ATOM	1642	OE2	GLU	A	206	13.005	19.777	59.194	1.00	35.12	AAAA
ATOM	1643	C	GLU	A	206	15.882	17.045	60.363	1.00	32.34	AAAA
ATOM	1644	O	GLU	A	206	16.209	15.909	60.706	1.00	31.83	AAAA
ATOM	1645	N	GLU	A	207	16.680	17.847	59.670	1.00	32.46	AAAA
ATOM	1646	CA	GLU	A	207	18.017	17.431	59.287	1.00	31.67	AAAA
ATOM	1647	CB	GLU	A	207	18.552	18.385	58.238	1.00	30.39	AAAA
ATOM	1648	CG	GLU	A	207	17.768	18.316	56.960	1.00	29.63	AAAA
ATOM	1649	CD	GLU	A	207	17.953	19.547	56.121	1.00	30.04	AAAA
ATOM	1650	OE1	GLU	A	207	19.108	19.991	55.971	1.00	30.31	AAAA

Figure 19-26

ATOM	1651	OE2	GLU	A	207	16.947	20.070	55.604	1.00	30.76	AAAA
ATOM	1652	C	GLU	A	207	18.879	17.433	60.537	1.00	32.04	AAAA
ATOM	1653	O	GLU	A	207	19.472	18.448	60.910	1.00	31.57	AAAA
ATOM	1654	N	ILE	A	208	18.935	16.272	61.178	1.00	32.57	AAAA
ATOM	1655	CA	ILE	A	208	19.674	16.111	62.408	1.00	33.37	AAAA
ATOM	1656	CB	ILE	A	208	18.709	15.647	63.519	1.00	33.65	AAAA
ATOM	1657	CG2	ILE	A	208	19.443	15.380	64.806	1.00	34.11	AAAA
ATOM	1658	CG1	ILE	A	208	17.673	16.742	63.757	1.00	33.94	AAAA
ATOM	1659	CD1	ILE	A	208	16.628	16.386	64.794	1.00	37.00	AAAA
ATOM	1660	C	ILE	A	208	20.863	15.174	62.280	1.00	34.00	AAAA
ATOM	1661	O	ILE	A	208	21.506	14.829	63.265	1.00	34.40	AAAA
ATOM	1662	N	GLY	A	209	21.177	14.768	61.062	1.00	34.64	AAAA
ATOM	1663	CA	GLY	A	209	22.321	13.903	60.913	1.00	35.55	AAAA
ATOM	1664	C	GLY	A	209	22.164	12.671	60.057	1.00	36.80	AAAA
ATOM	1665	O	GLY	A	209	21.148	12.461	59.400	1.00	37.32	AAAA
ATOM	1666	N	GLU	A	210	23.199	11.836	60.100	1.00	37.78	AAAA
ATOM	1667	CA	GLU	A	210	23.256	10.621	59.315	1.00	38.04	AAAA
ATOM	1668	CB	GLU	A	210	23.600	11.013	57.892	1.00	38.54	AAAA
ATOM	1669	CG	GLU	A	210	23.469	9.960	56.858	1.00	38.99	AAAA
ATOM	1670	CD	GLU	A	210	24.118	10.412	55.580	1.00	40.10	AAAA
ATOM	1671	OE1	GLU	A	210	25.365	10.437	55.555	1.00	40.86	AAAA
ATOM	1672	OE2	GLU	A	210	23.396	10.767	54.619	1.00	40.41	AAAA
ATOM	1673	C	GLU	A	210	24.377	9.770	59.894	1.00	37.98	AAAA
ATOM	1674	O	GLU	A	210	25.498	10.244	60.041	1.00	38.52	AAAA
ATOM	1675	N	GLY	A	211	24.085	8.517	60.220	1.00	38.02	AAAA
ATOM	1676	CA	GLY	A	211	25.116	7.654	60.770	1.00	38.09	AAAA
ATOM	1677	C	GLY	A	211	25.542	8.075	62.164	1.00	38.26	AAAA
ATOM	1678	O	GLY	A	211	24.697	8.443	62.977	1.00	37.82	AAAA
ATOM	1679	N	LYS	A	212	26.848	8.030	62.434	1.00	38.20	AAAA
ATOM	1680	CA	LYS	A	212	27.396	8.399	63.743	1.00	37.56	AAAA
ATOM	1681	CB	LYS	A	212	28.921	8.209	63.766	1.00	38.86	AAAA
ATOM	1682	CG	LYS	A	212	29.416	6.810	63.385	1.00	40.93	AAAA
ATOM	1683	CD	LYS	A	212	29.001	5.746	64.405	1.00	42.04	AAAA
ATOM	1684	CE	LYS	A	212	29.251	4.318	63.891	1.00	42.80	AAAA
ATOM	1685	NZ	LYS	A	212	30.673	4.002	63.562	1.00	42.32	AAAA
ATOM	1686	C	LYS	A	212	27.093	9.859	64.054	1.00	37.08	AAAA
ATOM	1687	O	LYS	A	212	27.075	10.269	65.218	1.00	36.94	AAAA
ATOM	1688	N	GLY	A	213	26.854	10.636	63.002	1.00	35.41	AAAA
ATOM	1689	CA	GLY	A	213	26.592	12.054	63.170	1.00	34.24	AAAA
ATOM	1690	C	GLY	A	213	25.163	12.438	63.470	1.00	33.27	AAAA
ATOM	1691	O	GLY	A	213	24.861	13.611	63.666	1.00	33.29	AAAA
ATOM	1692	N	LYS	A	214	24.280	11.451	63.512	1.00	31.79	AAAA
ATOM	1693	CA	LYS	A	214	22.883	11.710	63.794	1.00	30.47	AAAA
ATOM	1694	CB	LYS	A	214	22.111	10.396	63.737	1.00	30.35	AAAA
ATOM	1695	CG	LYS	A	214	20.676	10.552	63.280	1.00	30.45	AAAA
ATOM	1696	CD	LYS	A	214	20.141	9.241	62.759	1.00	29.75	AAAA
ATOM	1697	CE	LYS	A	214	18.737	9.400	62.229	1.00	30.19	AAAA
ATOM	1698	NZ	LYS	A	214	18.179	8.138	61.671	1.00	31.35	AAAA
ATOM	1699	C	LYS	A	214	22.778	12.374	65.168	1.00	30.31	AAAA
ATOM	1700	O	LYS	A	214	23.193	11.814	66.177	1.00	30.44	AAAA
ATOM	1701	N	GLY	A	215	22.243	13.590	65.192	1.00	29.95	AAAA
ATOM	1702	CA	GLY	A	215	22.128	14.325	66.437	1.00	29.16	AAAA
ATOM	1703	C	GLY	A	215	23.222	15.379	66.582	1.00	28.54	AAAA
ATOM	1704	O	GLY	A	215	23.306	16.061	67.602	1.00	28.27	AAAA
ATOM	1705	N	TYR	A	216	24.063	15.521	65.561	1.00	27.35	AAAA
ATOM	1706	CA	TYR	A	216	25.150	16.497	65.616	1.00	27.08	AAAA
ATOM	1707	CB	TYR	A	216	26.516	15.800	65.531	1.00	28.38	AAAA
ATOM	1708	CG	TYR	A	216	26.786	14.966	66.757	1.00	30.21	AAAA
ATOM	1709	CD1	TYR	A	216	26.138	13.735	66.955	1.00	29.81	AAAA
ATOM	1710	CE1	TYR	A	216	26.311	13.014	68.138	1.00	30.03	AAAA
ATOM	1711	CD2	TYR	A	216	27.619	15.450	67.774	1.00	29.71	AAAA
ATOM	1712	CE2	TYR	A	216	27.798	14.741	68.957	1.00	29.96	AAAA
ATOM	1713	CZ	TYR	A	216	27.143	13.528	69.138	1.00	30.84	AAAA
ATOM	1714	OH	TYR	A	216	27.297	12.859	70.332	1.00	31.14	AAAA
ATOM	1715	C	TYR	A	216	25.055	17.599	64.581	1.00	25.40	AAAA
ATOM	1716	O	TYR	A	216	26.046	18.240	64.243	1.00	26.38	AAAA

Figure 19-27

ATOM	1717	N	ASN	A	217	23.845	17.791	64.076	1.00	23.55	AAAA
ATOM	1718	CA	ASN	A	217	23.549	18.830	63.119	1.00	21.52	AAAA
ATOM	1719	CB	ASN	A	217	23.431	18.282	61.699	1.00	20.64	AAAA
ATOM	1720	CG	ASN	A	217	23.202	19.386	60.669	1.00	20.29	AAAA
ATOM	1721	OD1	ASN	A	217	22.089	19.888	60.499	1.00	18.03	AAAA
ATOM	1722	ND2	ASN	A	217	24.274	19.790	60.004	1.00	19.95	AAAA
ATOM	1723	C	ASN	A	217	22.216	19.346	63.605	1.00	21.64	AAAA
ATOM	1724	O	ASN	A	217	21.263	18.576	63.757	1.00	20.34	AAAA
ATOM	1725	N	LEU	A	218	22.165	20.647	63.873	1.00	22.22	AAAA
ATOM	1726	CA	LEU	A	218	20.960	21.282	64.388	1.00	22.03	AAAA
ATOM	1727	CB	LEU	A	218	21.195	21.711	65.840	1.00	20.97	AAAA
ATOM	1728	CG	LEU	A	218	20.051	21.838	66.841	1.00	20.94	AAAA
ATOM	1729	CD1	LEU	A	218	20.513	22.744	67.936	1.00	20.31	AAAA
ATOM	1730	CD2	LEU	A	218	18.818	22.412	66.227	1.00	21.27	AAAA
ATOM	1731	C	LEU	A	218	20.669	22.513	63.547	1.00	22.70	AAAA
ATOM	1732	O	LEU	A	218	21.451	23.454	63.557	1.00	22.64	AAAA
ATOM	1733	N	ASN	A	219	19.564	22.491	62.808	1.00	24.00	AAAA
ATOM	1734	CA	ASN	A	219	19.166	23.626	61.990	1.00	25.33	AAAA
ATOM	1735	CB	ASN	A	219	18.656	23.190	60.614	1.00	26.94	AAAA
ATOM	1736	CG	ASN	A	219	19.737	22.601	59.749	1.00	26.68	AAAA
ATOM	1737	OD1	ASN	A	219	20.812	23.169	59.626	1.00	28.06	AAAA
ATOM	1738	ND2	ASN	A	219	19.446	21.471	59.117	1.00	26.26	AAAA
ATOM	1739	C	ASN	A	219	18.046	24.345	62.710	1.00	25.69	AAAA
ATOM	1740	O	ASN	A	219	17.118	23.706	63.210	1.00	27.51	AAAA
ATOM	1741	N	ILE	A	220	18.122	25.667	62.753	1.00	25.05	AAAA
ATOM	1742	CA	ILE	A	220	17.107	26.457	63.428	1.00	25.87	AAAA
ATOM	1743	CB	ILE	A	220	17.733	27.331	64.557	1.00	25.04	AAAA
ATOM	1744	CG2	ILE	A	220	16.654	28.152	65.227	1.00	25.24	AAAA
ATOM	1745	CG1	ILE	A	220	18.460	26.447	65.584	1.00	24.07	AAAA
ATOM	1746	CD1	ILE	A	220	17.557	25.502	66.378	1.00	22.28	AAAA
ATOM	1747	C	ILE	A	220	16.430	27.370	62.414	1.00	26.20	AAAA
ATOM	1748	O	ILE	A	220	16.801	28.534	62.265	1.00	25.35	AAAA
ATOM	1749	N	PRO	A	221	15.421	26.850	61.704	1.00	26.70	AAAA
ATOM	1750	CD	PRO	A	221	14.840	25.501	61.778	1.00	27.17	AAAA
ATOM	1751	CA	PRO	A	221	14.706	27.640	60.703	1.00	27.67	AAAA
ATOM	1752	CB	PRO	A	221	13.771	26.613	60.064	1.00	26.81	AAAA
ATOM	1753	CG	PRO	A	221	14.473	25.293	60.346	1.00	27.36	AAAA
ATOM	1754	C	PRO	A	221	13.944	28.763	61.390	1.00	28.61	AAAA
ATOM	1755	O	PRO	A	221	13.218	28.515	62.363	1.00	29.91	AAAA
ATOM	1756	N	LEU	A	222	14.100	29.990	60.900	1.00	28.15	AAAA
ATOM	1757	CA	LEU	A	222	13.408	31.117	61.511	1.00	28.48	AAAA
ATOM	1758	CB	LEU	A	222	14.431	32.041	62.191	1.00	28.69	AAAA
ATOM	1759	CG	LEU	A	222	15.187	31.394	63.371	1.00	28.67	AAAA
ATOM	1760	CD1	LEU	A	222	16.304	32.300	63.837	1.00	28.62	AAAA
ATOM	1761	CD2	LEU	A	222	14.231	31.106	64.527	1.00	27.65	AAAA
ATOM	1762	C	LEU	A	222	12.726	31.882	60.518	1.00	28.44	AAAA
ATOM	1763	O	LEU	A	222	12.118	31.958	59.325	1.00	27.90	AAAA
ATOM	1764	N	PRO	A	223	11.113	32.441	61.009	1.00	28.79	AAAA
ATOM	1765	CD	PRO	A	223	10.966	32.357	62.410	1.00	29.20	AAAA
ATOM	1766	CA	PRO	A	223	10.437	33.202	60.227	1.00	29.36	AAAA
ATOM	1767	CB	PRO	A	223	9.256	33.287	61.183	1.00	28.98	AAAA
ATOM	1768	CG	PRO	A	223	9.965	33.502	62.485	1.00	28.68	AAAA
ATOM	1769	C	PRO	A	223	10.890	34.585	59.753	1.00	30.15	AAAA
ATOM	1770	O	PRO	A	223	11.864	35.152	60.253	1.00	30.18	AAAA
ATOM	1771	N	LYS	A	224	10.150	35.112	58.781	1.00	30.50	AAAA
ATOM	1772	CA	LYS	A	224	10.398	36.422	58.213	1.00	29.92	AAAA
ATOM	1773	CB	LYS	A	224	9.491	36.661	57.008	1.00	30.57	AAAA
ATOM	1774	CG	LYS	A	224	9.588	35.676	55.893	1.00	30.06	AAAA
ATOM	1775	CD	LYS	A	224	8.640	36.087	54.798	1.00	30.91	AAAA
ATOM	1776	CE	LYS	A	224	8.575	35.051	53.705	1.00	32.15	AAAA
ATOM	1777	NZ	LYS	A	224	7.628	35.476	52.648	1.00	32.75	AAAA
ATOM	1778	C	LYS	A	224	10.050	37.468	59.260	1.00	29.75	AAAA
ATOM	1779	O	LYS	A	224	9.308	37.193	60.196	1.00	29.84	AAAA
ATOM	1780	N	GLY	A	225	10.555	38.678	59.079	1.00	29.39	AAAA
ATOM	1781	CA	GLY	A	225	10.261	39.730	60.031	1.00	29.87	AAAA
ATOM	1782	C	GLY	A	225	10.809	39.447	61.415	1.00	29.85	AAAA

Figure 19-28

ATOM	1783	O	GLY	A	225	10.371	40.051	62.392	1.00	29.85	AAAA
ATOM	1784	N	LEU	A	226	11.775	38.536	61.499	1.00	29.50	AAAA
ATOM	1785	CA	LEU	A	226	12.374	38.175	62.778	1.00	29.80	AAAA
ATOM	1786	CB	LEU	A	226	13.513	37.170	62.570	1.00	28.81	AAAA
ATOM	1787	CG	LEU	A	226	14.097	36.514	63.820	1.00	27.29	AAAA
ATOM	1788	CD1	LEU	A	226	13.132	35.452	64.275	1.00	26.06	AAAA
ATOM	1789	CD2	LEU	A	226	15.455	35.888	63.538	1.00	27.03	AAAA
ATOM	1790	C	LEU	A	226	12.936	39.428	63.448	1.00	30.68	AAAA
ATOM	1791	O	LEU	A	226	13.636	40.217	62.804	1.00	30.57	AAAA
ATOM	1792	N	ASN	A	227	12.624	39.617	64.729	1.00	31.46	AAAA
ATOM	1793	CA	ASN	A	227	13.139	40.769	65.469	1.00	32.06	AAAA
ATOM	1794	CB	ASN	A	227	12.012	41.507	66.217	1.00	31.74	AAAA
ATOM	1795	CG	ASN	A	227	11.291	40.630	67.234	1.00	32.07	AAAA
ATOM	1796	OD1	ASN	A	227	11.914	40.017	68.104	1.00	31.61	AAAA
ATOM	1797	ND2	ASN	A	227	9.962	40.592	67.141	1.00	31.59	AAAA
ATOM	1798	C	ASN	A	227	14.225	40.334	66.444	1.00	32.45	AAAA
ATOM	1799	O	ASN	A	227	14.413	39.140	66.688	1.00	32.78	AAAA
ATOM	1800	N	ASP	A	228	14.943	41.297	67.002	1.00	33.32	AAAA
ATOM	1801	CA	ASP	A	228	16.017	40.976	67.928	1.00	34.75	AAAA
ATOM	1802	CB	ASP	A	228	16.508	42.233	68.654	1.00	36.77	AAAA
ATOM	1803	CG	ASP	A	228	17.154	43.238	67.714	1.00	37.28	AAAA
ATOM	1804	OD1	ASP	A	228	17.662	42.816	66.652	1.00	37.78	AAAA
ATOM	1805	OD2	ASP	A	228	17.180	44.443	68.054	1.00	37.21	AAAA
ATOM	1806	C	ASP	A	228	15.707	39.892	68.964	1.00	34.93	AAAA
ATOM	1807	O	ASP	A	228	16.448	38.919	69.056	1.00	36.92	AAAA
ATOM	1808	N	ASN	A	229	14.635	40.054	69.741	1.00	33.90	AAAA
ATOM	1809	CA	ASN	A	229	14.268	39.079	70.775	1.00	33.01	AAAA
ATOM	1810	CB	ASN	A	229	12.965	39.481	71.455	1.00	33.79	AAAA
ATOM	1811	CG	ASN	A	229	13.131	40.663	72.369	1.00	34.04	AAAA
ATOM	1812	OD1	ASN	A	229	13.783	40.564	73.405	1.00	34.25	AAAA
ATOM	1813	ND2	ASN	A	229	12.550	41.797	71.988	1.00	34.05	AAAA
ATOM	1814	C	ASN	A	229	14.114	37.656	70.276	1.00	32.98	AAAA
ATOM	1815	O	ASN	A	229	14.529	36.697	70.944	1.00	32.77	AAAA
ATOM	1816	N	GLU	A	230	13.496	37.523	69.108	1.00	32.02	AAAA
ATOM	1817	CA	GLU	A	230	13.277	36.227	68.516	1.00	30.72	AAAA
ATOM	1818	CB	GLU	A	230	12.399	36.375	67.272	1.00	31.38	AAAA
ATOM	1819	CG	GLU	A	230	11.006	36.896	67.583	1.00	31.02	AAAA
ATOM	1820	CD	GLU	A	230	10.175	37.187	66.350	1.00	31.52	AAAA
ATOM	1821	OE1	GLU	A	230	10.644	37.970	65.497	1.00	31.89	AAAA
ATOM	1822	OE2	GLU	A	230	9.047	36.655	66.241	1.00	31.04	AAAA
ATOM	1823	C	GLU	A	230	14.628	35.622	68.180	1.00	30.79	AAAA
ATOM	1824	O	GLU	A	230	14.905	34.465	68.512	1.00	31.05	AAAA
ATOM	1825	N	PHE	A	231	15.490	36.412	67.553	1.00	30.05	AAAA
ATOM	1826	CA	PHE	A	231	16.811	35.920	67.191	1.00	28.94	AAAA
ATOM	1827	CB	PHE	A	231	17.632	37.015	66.528	1.00	29.33	AAAA
ATOM	1828	CG	PHE	A	231	18.949	36.537	65.972	1.00	28.79	AAAA
ATOM	1829	CD1	PHE	A	231	18.982	35.585	64.957	1.00	28.93	AAAA
ATOM	1830	CD2	PHE	A	231	20.152	37.067	66.436	1.00	28.55	AAAA
ATOM	1831	CE1	PHE	A	231	20.195	35.160	64.397	1.00	28.32	AAAA
ATOM	1832	CE2	PHE	A	231	21.376	36.657	65.888	1.00	28.97	AAAA
ATOM	1833	CZ	PHE	A	231	21.397	35.695	64.860	1.00	28.81	AAAA
ATOM	1834	C	PHE	A	231	17.559	35.443	68.413	1.00	28.25	AAAA
ATOM	1835	O	PHE	A	231	17.999	34.302	68.485	1.00	27.97	AAAA
ATOM	1836	N	LEU	A	232	17.691	36.329	69.384	1.00	27.93	AAAA
ATOM	1837	CA	LEU	A	232	18.425	36.003	70.590	1.00	27.93	AAAA
ATOM	1838	CB	LEU	A	232	18.521	37.234	71.484	1.00	28.16	AAAA
ATOM	1839	CG	LEU	A	232	19.220	38.379	70.747	1.00	27.96	AAAA
ATOM	1840	CD1	LEU	A	232	19.203	39.629	71.587	1.00	27.57	AAAA
ATOM	1841	CD2	LEU	A	232	20.639	37.955	70.387	1.00	27.76	AAAA
ATOM	1842	C	LEU	A	232	17.815	34.851	71.340	1.00	27.95	AAAA
ATOM	1843	O	LEU	A	232	18.526	34.061	71.941	1.00	27.92	AAAA
ATOM	1844	N	PHE	A	233	16.495	34.758	71.298	1.00	28.81	AAAA
ATOM	1845	CA	PHE	A	233	15.786	33.685	71.972	1.00	30.27	AAAA
ATOM	1846	CB	PHE	A	233	14.278	33.837	71.745	1.00	31.51	AAAA
ATOM	1847	CG	PHE	A	233	13.465	32.710	72.308	1.00	32.38	AAAA
ATOM	1848	CD1	PHE	A	233	13.257	32.599	73.677	1.00	33.66	AAAA

Figure 19-29

ATOM	1849	CD2	PHE	A	233	12.928	31.741	71.467	1.00	33.51	AAAA
ATOM	1850	CE1	PHE	A	233	12.518	31.537	74.201	1.00	35.10	AAAA
ATOM	1851	CE2	PHE	A	233	12.193	30.677	71.975	1.00	34.21	AAAA
ATOM	1852	CZ	PHE	A	233	11.986	30.572	73.344	1.00	35.23	AAAA
ATOM	1853	C	PHE	A	233	16.219	32.301	71.483	1.00	30.55	AAAA
ATOM	1854	O	PHE	A	233	16.438	31.391	72.280	1.00	30.65	AAAA
ATOM	1855	N	ALA	A	234	16.317	32.151	70.165	1.00	30.21	AAAA
ATOM	1856	CA	ALA	A	234	16.698	30.892	69.549	1.00	28.97	AAAA
ATOM	1857	CB	ALA	A	234	16.398	30.942	68.065	1.00	30.40	AAAA
ATOM	1858	C	ALA	A	234	18.169	30.571	69.761	1.00	28.27	AAAA
ATOM	1859	O	ALA	A	234	18.564	29.401	69.830	1.00	26.69	AAAA
ATOM	1860	N	LEU	A	235	18.978	31.614	69.855	1.00	27.56	AAAA
ATOM	1861	CA	LEU	A	235	20.402	31.427	70.055	1.00	29.17	AAAA
ATOM	1862	CB	LEU	A	235	21.126	32.767	69.989	1.00	29.04	AAAA
ATOM	1863	CG	LEU	A	235	22.527	32.757	69.378	1.00	28.54	AAAA
ATOM	1864	CD1	LEU	A	235	23.350	33.837	70.058	1.00	27.05	AAAA
ATOM	1865	CD2	LEU	A	235	23.182	31.408	69.558	1.00	27.21	AAAA
ATOM	1866	C	LEU	A	235	20.637	30.799	71.429	1.00	30.99	AAAA
ATOM	1867	O	LEU	A	235	21.159	29.697	71.547	1.00	31.65	AAAA
ATOM	1868	N	GLU	A	236	20.242	31.514	72.471	1.00	31.88	AAAA
ATOM	1869	CA	GLU	A	236	20.409	31.042	73.838	1.00	32.99	AAAA
ATOM	1870	CB	GLU	A	236	19.689	31.990	74.790	1.00	34.63	AAAA
ATOM	1871	CG	GLU	A	236	19.980	33.449	74.531	1.00	36.79	AAAA
ATOM	1872	CD	GLU	A	236	19.044	34.360	75.294	1.00	38.99	AAAA
ATOM	1873	OE1	GLU	A	236	17.803	34.303	75.070	1.00	39.03	AAAA
ATOM	1874	OE2	GLU	A	236	19.559	35.132	76.126	1.00	41.56	AAAA
ATOM	1875	C	GLU	A	236	19.806	29.656	73.982	1.00	32.94	AAAA
ATOM	1876	O	GLU	A	236	20.379	28.753	74.595	1.00	31.76	AAAA
ATOM	1877	N	LYS	A	237	18.631	29.503	73.399	1.00	32.83	AAAA
ATOM	1878	CA	LYS	A	237	17.906	28.256	73.471	1.00	33.59	AAAA
ATOM	1879	CB	LYS	A	237	16.504	28.506	72.942	1.00	35.00	AAAA
ATOM	1880	CG	LYS	A	237	15.516	27.436	73.213	1.00	36.69	AAAA
ATOM	1881	CD	LYS	A	237	14.310	28.008	73.940	1.00	38.53	AAAA
ATOM	1882	CE	LYS	A	237	14.636	28.331	75.392	1.00	39.27	AAAA
ATOM	1883	NZ	LYS	A	237	13.398	28.531	76.204	1.00	39.42	AAAA
ATOM	1884	C	LYS	A	237	18.619	27.129	72.707	1.00	33.14	AAAA
ATOM	1885	O	LYS	A	237	18.850	26.051	73.260	1.00	33.29	AAAA
ATOM	1886	N	SER	A	238	18.985	27.374	71.452	1.00	32.13	AAAA
ATOM	1887	CA	SER	A	238	19.671	26.345	70.685	1.00	31.25	AAAA
ATOM	1888	CB	SER	A	238	19.740	26.717	69.194	1.00	30.52	AAAA
ATOM	1889	OG	SER	A	238	20.544	27.851	68.970	1.00	29.95	AAAA
ATOM	1890	C	SER	A	238	21.075	26.064	71.236	1.00	31.21	AAAA
ATOM	1891	O	SER	A	238	21.556	24.929	71.169	1.00	30.06	AAAA
ATOM	1892	N	LEU	A	239	21.740	27.077	71.782	1.00	31.71	AAAA
ATOM	1893	CA	LEU	A	239	23.070	26.842	72.351	1.00	33.47	AAAA
ATOM	1894	CB	LEU	A	239	23.698	28.130	72.900	1.00	31.25	AAAA
ATOM	1895	CG	LEU	A	239	23.988	29.300	71.977	1.00	29.80	AAAA
ATOM	1896	CD1	LEU	A	239	24.589	30.410	72.787	1.00	29.05	AAAA
ATOM	1897	CD2	LEU	A	239	24.919	28.903	70.872	1.00	29.36	AAAA
ATOM	1898	C	LEU	A	239	22.933	25.839	73.502	1.00	35.41	AAAA
ATOM	1899	O	LEU	A	239	23.812	25.012	73.735	1.00	36.25	AAAA
ATOM	1900	N	GLU	A	240	21.816	25.906	74.213	1.00	37.34	AAAA
ATOM	1901	CA	GLU	A	240	21.594	25.005	75.331	1.00	39.39	AAAA
ATOM	1902	CB	GLU	A	240	20.281	25.361	76.017	1.00	41.90	AAAA
ATOM	1903	CG	GLU	A	240	20.040	24.610	77.308	1.00	45.52	AAAA
ATOM	1904	CD	GLU	A	240	19.665	25.552	78.432	1.00	47.80	AAAA
ATOM	1905	OE1	GLU	A	240	18.670	26.295	78.274	1.00	49.70	AAAA
ATOM	1906	OE2	GLU	A	240	20.364	25.559	79.469	1.00	48.04	AAAA
ATOM	1907	C	GLU	A	240	21.583	23.555	74.875	1.00	38.80	AAAA
ATOM	1908	O	GLU	A	240	22.224	22.700	75.478	1.00	37.85	AAAA
ATOM	1909	N	ILE	A	241	20.847	23.293	73.804	1.00	39.66	AAAA
ATOM	1910	CA	ILE	A	241	20.751	21.955	73.223	1.00	40.81	AAAA
ATOM	1911	CB	ILE	A	241	19.912	21.994	71.917	1.00	41.10	AAAA
ATOM	1912	CG2	ILE	A	241	19.850	20.621	71.287	1.00	40.88	AAAA
ATOM	1913	CG1	ILE	A	241	18.502	22.514	72.220	1.00	41.45	AAAA
ATOM	1914	CD1	ILE	A	241	17.641	22.745	70.992	1.00	41.14	AAAA

Figure 19-30

ATOM	1915	C	ILE A	241	22.159	21.424	72.893	1.00	41.66	AAAA
ATOM	1916	O	ILE A	241	22.445	20.229	73.045	1.00	42.10	AAAA
ATOM	1917	N	VAL A	242	23.026	22.324	72.432	1.00	41.42	AAAA
ATOM	1918	CA	VAL A	242	24.394	21.977	72.076	1.00	41.23	AAAA
ATOM	1919	CB	VAL A	242	25.089	23.146	71.351	1.00	40.40	AAAA
ATOM	1920	CG1	VAL A	242	26.556	22.850	71.171	1.00	39.25	AAAA
ATOM	1921	CG2	VAL A	242	24.438	23.384	70.004	1.00	39.79	AAAA
ATOM	1922	C	VAL A	242	25.228	21.604	73.298	1.00	42.67	AAAA
ATOM	1923	O	VAL A	242	25.882	20.562	73.316	1.00	41.83	AAAA
ATOM	1924	N	LYS A	243	25.198	22.456	74.318	1.00	44.41	AAAA
ATOM	1925	CA	LYS A	243	25.972	22.215	75.523	1.00	46.51	AAAA
ATOM	1926	CB	LYS A	243	25.797	23.363	76.522	1.00	47.29	AAAA
ATOM	1927	CG	LYS A	243	26.820	23.312	77.564	1.00	48.40	AAAA
ATOM	1928	CD	LYS A	243	26.479	24.248	78.823	1.00	48.88	AAAA
ATOM	1929	CE	LYS A	243	26.355	25.691	78.380	1.00	49.62	AAAA
ATOM	1930	NZ	LYS A	243	25.926	26.576	79.505	1.00	50.11	AAAA
ATOM	1931	C	LYS A	243	25.639	20.891	76.209	1.00	47.59	AAAA
ATOM	1932	O	LYS A	243	26.537	20.216	76.711	1.00	48.17	AAAA
ATOM	1933	N	GLU A	244	24.362	20.517	76.237	1.00	48.86	AAAA
ATOM	1934	CA	GLU A	244	23.957	19.262	76.877	1.00	50.82	AAAA
ATOM	1935	CB	GLU A	244	22.432	19.208	77.103	1.00	52.08	AAAA
ATOM	1936	CG	GLU A	244	21.818	20.405	77.829	1.00	53.82	AAAA
ATOM	1937	CD	GLU A	244	20.359	20.174	78.230	1.00	54.49	AAAA
ATOM	1938	OE1	GLU A	244	19.666	21.158	78.595	1.00	55.15	AAAA
ATOM	1939	OE2	GLU A	244	19.912	19.006	78.200	1.00	54.98	AAAA
ATOM	1940	C	GLU A	244	24.338	18.046	76.033	1.00	51.06	AAAA
ATOM	1941	O	GLU A	244	24.206	16.905	76.477	1.00	51.68	AAAA
ATOM	1942	N	VAL A	245	24.810	18.292	74.820	1.00	51.12	AAAA
ATOM	1943	CA	VAL A	245	25.149	17.212	73.904	1.00	50.08	AAAA
ATOM	1944	CB	VAL A	245	24.217	17.263	72.677	1.00	50.22	AAAA
ATOM	1945	CG1	VAL A	245	24.615	16.217	71.651	1.00	51.07	AAAA
ATOM	1946	CG2	VAL A	245	22.794	17.049	73.118	1.00	50.79	AAAA
ATOM	1947	C	VAL A	245	26.578	17.254	73.397	1.00	49.43	AAAA
ATOM	1948	O	VAL A	245	27.101	16.250	72.917	1.00	48.65	AAAA
ATOM	1949	N	PHE A	246	27.220	18.408	73.522	1.00	48.65	AAAA
ATOM	1950	CA	PHE A	246	28.556	18.552	72.982	1.00	47.97	AAAA
ATOM	1951	CB	PHE A	246	28.420	19.212	71.607	1.00	46.45	AAAA
ATOM	1952	CG	PHE A	246	29.553	18.932	70.671	1.00	45.35	AAAA
ATOM	1953	CD1	PHE A	246	29.841	17.629	70.280	1.00	44.13	AAAA
ATOM	1954	CD2	PHE A	246	30.291	19.972	70.124	1.00	44.40	AAAA
ATOM	1955	CE1	PHE A	246	30.840	17.370	69.356	1.00	43.95	AAAA
ATOM	1956	CE2	PHE A	246	31.292	19.721	69.197	1.00	43.47	AAAA
ATOM	1957	CZ	PHE A	246	31.566	18.422	68.811	1.00	44.05	AAAA
ATOM	1958	C	PHE A	246	29.481	19.383	73.860	1.00	48.60	AAAA
ATOM	1959	O	PHE A	246	29.132	20.501	74.239	1.00	49.59	AAAA
ATOM	1960	N	GLU A	247	30.647	18.834	74.198	1.00	48.69	AAAA
ATOM	1961	CA	GLU A	247	31.644	19.578	74.977	1.00	49.45	AAAA
ATOM	1962	CB	GLU A	247	32.174	18.768	76.178	1.00	51.91	AAAA
ATOM	1963	CG	GLU A	247	31.257	18.659	77.398	1.00	54.39	AAAA
ATOM	1964	CD	GLU A	247	29.986	17.845	77.146	1.00	57.34	AAAA
ATOM	1965	OE1	GLU A	247	29.100	18.315	76.393	1.00	58.48	AAAA
ATOM	1966	OE2	GLU A	247	29.877	16.725	77.702	1.00	57.95	AAAA
ATOM	1967	C	GLU A	247	32.807	19.903	74.024	1.00	47.39	AAAA
ATOM	1968	O	GLU A	247	33.742	19.119	73.872	1.00	46.65	AAAA
ATOM	1969	N	PRO A	248	32.748	21.070	73.371	1.00	46.25	AAAA
ATOM	1970	CD	PRO A	248	31.651	22.033	73.543	1.00	46.49	AAAA
ATOM	1971	CA	PRO A	248	33.710	21.614	72.411	1.00	45.44	AAAA
ATOM	1972	CB	PRO A	248	33.063	22.948	72.017	1.00	45.57	AAAA
ATOM	1973	CG	PRO A	248	31.604	22.661	72.178	1.00	46.28	AAAA
ATOM	1974	C	PRO A	248	35.155	21.814	72.880	1.00	44.29	AAAA
ATOM	1975	O	PRO A	248	35.401	22.370	73.947	1.00	44.57	AAAA
ATOM	1976	N	GLU A	249	36.100	21.364	72.059	1.00	42.21	AAAA
ATOM	1977	CA	GLU A	249	37.522	21.526	72.340	1.00	39.87	AAAA
ATOM	1978	CB	GLU A	249	38.344	20.460	71.625	1.00	39.58	AAAA
ATOM	1979	CG	GLU A	249	37.960	19.030	71.957	1.00	41.32	AAAA
ATOM	1980	CD	GLU A	249	38.825	18.007	71.241	1.00	40.96	AAAA

ATOM	1981	OE1	GLU	A	249	38.871	18.017	69.996	1.00	41.55	AAAA
ATOM	1982	OE2	GLU	A	249	39.462	17.187	71.926	1.00	42.49	AAAA
ATOM	1983	C	GLU	A	249	37.840	22.873	71.718	1.00	38.81	AAAA
ATOM	1984	O	GLU	A	249	38.715	23.617	72.181	1.00	38.27	AAAA
ATOM	1985	N	VAL	A	250	37.109	23.160	70.644	1.00	36.60	AAAA
ATOM	1986	CA	VAL	A	250	37.242	24.402	69.890	1.00	34.20	AAAA
ATOM	1987	CB	VAL	A	250	38.379	24.321	68.862	1.00	33.73	AAAA
ATOM	1988	CG1	VAL	A	250	38.085	23.209	67.864	1.00	33.26	AAAA
ATOM	1989	CG2	VAL	A	250	38.546	25.678	68.153	1.00	33.75	AAAA
ATOM	1990	C	VAL	A	250	35.945	24.617	69.130	1.00	31.98	AAAA
ATOM	1991	O	VAL	A	250	35.205	23.658	68.904	1.00	32.36	AAAA
ATOM	1992	N	TYR	A	251	35.657	25.863	68.760	1.00	28.65	AAAA
ATOM	1993	CA	TYR	A	251	34.449	26.150	67.991	1.00	26.49	AAAA
ATOM	1994	CB	TYR	A	251	33.241	26.442	68.906	1.00	24.32	AAAA
ATOM	1995	CG	TYR	A	251	33.193	27.853	69.465	1.00	22.96	AAAA
ATOM	1996	CD1	TYR	A	251	32.771	28.931	68.668	1.00	22.21	AAAA
ATOM	1997	CE1	TYR	A	251	32.791	30.234	69.151	1.00	21.29	AAAA
ATOM	1998	CD2	TYR	A	251	33.628	28.124	70.771	1.00	21.47	AAAA
ATOM	1999	CE2	TYR	A	251	33.651	29.425	71.265	1.00	20.80	AAAA
ATOM	2000	CZ	TYR	A	251	33.237	30.475	70.449	1.00	20.77	AAAA
ATOM	2001	OH	TYR	A	251	33.309	31.768	70.913	1.00	21.41	AAAA
ATOM	2002	C	TYR	A	251	34.691	27.345	67.092	1.00	24.59	AAAA
ATOM	2003	O	TYR	A	251	35.504	28.216	67.410	1.00	25.87	AAAA
ATOM	2004	N	LEU	A	252	33.984	27.374	65.970	1.00	22.49	AAAA
ATOM	2005	CA	LEU	A	252	34.082	28.482	65.045	1.00	20.96	AAAA
ATOM	2006	CB	LEU	A	252	34.523	28.018	63.657	1.00	21.31	AAAA
ATOM	2007	CG	LEU	A	252	35.940	27.472	63.556	1.00	21.03	AAAA
ATOM	2008	CD1	LEU	A	252	35.947	26.028	63.977	1.00	22.16	AAAA
ATOM	2009	CD2	LEU	A	252	36.440	27.594	62.143	1.00	22.13	AAAA
ATOM	2010	C	LEU	A	252	32.731	29.159	64.959	1.00	19.60	AAAA
ATOM	2011	O	LEU	A	252	31.689	28.523	65.070	1.00	19.95	AAAA
ATOM	2012	N	LEU	A	253	32.748	30.461	64.756	1.00	17.95	AAAA
ATOM	2013	CA	LEU	A	253	31.521	31.222	64.675	1.00	17.33	AAAA
ATOM	2014	CB	LEU	A	253	31.441	32.142	65.900	1.00	16.31	AAAA
ATOM	2015	CG	LEU	A	253	30.266	33.070	66.153	1.00	15.81	AAAA
ATOM	2016	CD1	LEU	A	253	28.990	32.267	66.377	1.00	14.74	AAAA
ATOM	2017	CD2	LEU	A	253	30.602	33.925	67.368	1.00	15.83	AAAA
ATOM	2018	C	LEU	A	253	31.564	32.035	63.386	1.00	16.60	AAAA
ATOM	2019	O	LEU	A	253	32.548	32.722	63.132	1.00	16.40	AAAA
ATOM	2020	N	GLN	A	254	30.526	31.936	62.557	1.00	15.88	AAAA
ATOM	2021	CA	GLN	A	254	30.507	32.716	61.328	1.00	16.27	AAAA
ATOM	2022	CB	GLN	A	254	30.045	31.881	60.121	1.00	15.88	AAAA
ATOM	2023	CG	GLN	A	254	28.587	32.048	59.734	1.00	18.52	AAAA
ATOM	2024	CD	GLN	A	254	28.380	32.935	58.519	1.00	17.54	AAAA
ATOM	2025	OE1	GLN	A	254	28.714	32.572	57.391	1.00	15.89	AAAA
ATOM	2026	NE2	GLN	A	254	27.828	34.103	58.750	1.00	18.49	AAAA
ATOM	2027	C	GLN	A	254	29.527	33.825	61.650	1.00	16.91	AAAA
ATOM	2028	O	GLN	A	254	28.450	33.571	62.198	1.00	17.41	AAAA
ATOM	2029	N	LEU	A	255	29.911	35.053	61.319	1.00	16.68	AAAA
ATOM	2030	CA	LEU	A	255	29.102	36.215	61.619	1.00	16.42	AAAA
ATOM	2031	CB	LEU	A	255	29.861	37.080	62.616	1.00	14.93	AAAA
ATOM	2032	CG	LEU	A	255	30.269	36.301	63.860	1.00	13.90	AAAA
ATOM	2033	CD1	LEU	A	255	31.494	36.924	64.515	1.00	12.24	AAAA
ATOM	2034	CD2	LEU	A	255	29.083	36.202	64.774	1.00	12.80	AAAA
ATOM	2035	C	LEU	A	255	28.699	37.048	60.404	1.00	18.32	AAAA
ATOM	2036	O	LEU	A	255	29.170	38.177	60.216	1.00	17.59	AAAA
ATOM	2037	N	GLY	A	256	27.813	36.482	59.588	1.00	19.75	AAAA
ATOM	2038	CA	GLY	A	256	27.322	37.188	58.422	1.00	20.77	AAAA
ATOM	2039	C	GLY	A	256	26.422	38.302	58.927	1.00	21.73	AAAA
ATOM	2040	O	GLY	A	256	25.642	38.096	59.857	1.00	21.38	AAAA
ATOM	2041	N	THR	A	257	26.528	39.485	58.325	1.00	22.82	AAAA
ATOM	2042	CA	THR	A	257	25.721	40.622	58.746	1.00	23.85	AAAA
ATOM	2043	CB	THR	A	257	26.460	41.968	58.549	1.00	23.99	AAAA
ATOM	2044	OG1	THR	A	257	26.729	42.169	57.153	1.00	25.54	AAAA
ATOM	2045	CG2	THR	A	257	27.780	41.985	59.329	1.00	24.07	AAAA
ATOM	2046	C	THR	A	257	24.438	40.691	57.948	1.00	24.97	AAAA

247/263
Figure 19-32

ATOM	2047	O	THR	A	257	23.692	41.672	58.048	1.00	25.84	AAAA
ATOM	2048	N	ASP	A	258	24.152	39.665	57.154	1.00	25.18	AAAA
ATOM	2049	CA	ASP	A	258	22.935	39.753	56.379	1.00	26.18	AAAA
ATOM	2050	CB	ASP	A	258	22.950	38.830	55.149	1.00	25.52	AAAA
ATOM	2051	CG	ASP	A	258	23.211	37.392	55.494	1.00	26.33	AAAA
ATOM	2052	C	ASP	A	258	21.649	39.574	57.178	1.00	26.74	AAAA
ATOM	2053	O	ASP	A	258	20.571	39.823	56.643	1.00	26.57	AAAA
ATOM	2054	OD1	ASP	A	258	23.014	37.029	56.675	1.00	26.85	AAAA
ATOM	2055	OD2	ASP	A	258	23.585	36.623	54.572	1.00	24.06	AAAA
ATOM	2056	N	PRO	A	259	21.727	39.114	58.449	1.00	26.95	AAAA
ATOM	2057	CD	PRO	A	259	22.834	38.589	59.271	1.00	27.34	AAAA
ATOM	2058	CA	PRO	A	259	20.467	38.976	59.190	1.00	27.05	AAAA
ATOM	2059	CB	PRO	A	259	20.886	38.186	60.425	1.00	26.38	AAAA
ATOM	2060	CG	PRO	A	259	22.247	38.718	60.669	1.00	27.84	AAAA
ATOM	2061	C	PRO	A	259	19.914	40.365	59.543	1.00	27.32	AAAA
ATOM	2062	O	PRO	A	259	18.739	40.510	59.871-	1.00	27.29	AAAA
ATOM	2063	N	LEU	A	260	20.771	41.383	59.452	1.00	26.97	AAAA
ATOM	2064	CA	LEU	A	260	20.389	42.763	59.752	1.00	26.74	AAAA
ATOM	2065	CB	LEU	A	260	21.621	43.680	59.680	1.00	27.21	AAAA
ATOM	2066	CG	LEU	A	260	22.732	43.465	60.709	1.00	27.01	AAAA
ATOM	2067	CD1	LEU	A	260	23.889	44.380	60.408	1.00	25.51	AAAA
ATOM	2068	CD2	LEU	A	260	22.189	43.718	62.112	1.00	27.39	AAAA
ATOM	2069	C	LEU	A	260	19.295	43.351	58.865	1.00	26.47	AAAA
ATOM	2070	O	LEU	A	260	19.278	43.137	57.649	1.00	26.72	AAAA
ATOM	2071	N	LEU	A	261	18.413	44.126	59.494	1.00	26.32	AAAA
ATOM	2072	CA	LEU	A	261	17.283	44.808	58.846	1.00	27.20	AAAA
ATOM	2073	CB	LEU	A	261	16.732	45.885	59.780	1.00	28.71	AAAA
ATOM	2074	CG	LEU	A	261	15.644	46.789	59.190	1.00	29.24	AAAA
ATOM	2075	CD1	LEU	A	261	14.433	45.954	58.883	1.00	29.44	AAAA
ATOM	2076	CD2	LEU	A	261	15.284	47.906	60.162	1.00	29.72	AAAA
ATOM	2077	C	LEU	A	261	17.506	45.454	57.473	1.00	27.90	AAAA
ATOM	2078	O	LEU	A	261	16.675	45.294	56.577	1.00	28.21	AAAA
ATOM	2079	N	GLU	A	262	18.597	46.202	57.310	1.00	27.61	AAAA
ATOM	2080	CA	GLU	A	262	18.887	46.877	56.043	1.00	26.92	AAAA
ATOM	2081	CB	GLU	A	262	19.949	47.955	56.241	1.00	25.85	AAAA
ATOM	2082	CG	GLU	A	262	19.549	49.119	57.117	1.00	25.36	AAAA
ATOM	2083	CD	GLU	A	262	19.552	48.787	58.580	1.00	25.78	AAAA
ATOM	2084	OE1	GLU	A	262	19.859	47.631	58.938	1.00	24.64	AAAA
ATOM	2085	OE2	GLU	A	262	19.255	49.694	59.381	1.00	25.82	AAAA
ATOM	2086	C	GLU	A	262	19.346	45.995	54.882	1.00	28.79	AAAA
ATOM	2087	O	GLU	A	262	19.354	46.439	53.724	1.00	28.70	AAAA
ATOM	2088	N	ASP	A	263	19.743	44.758	55.179	1.00	29.57	AAAA
ATOM	2089	CA	ASP	A	263	20.230	43.853	54.145	1.00	28.99	AAAA
ATOM	2090	CB	ASP	A	263	21.160	42.802	54.760	1.00	27.89	AAAA
ATOM	2091	CG	ASP	A	263	21.986	42.062	53.714	1.00	29.02	AAAA
ATOM	2092	OD1	ASP	A	263	23.194	41.863	53.957	1.00	28.06	AAAA
ATOM	2093	OD2	ASP	A	263	21.438	41.663	52.660	1.00	28.80	AAAA
ATOM	2094	C	ASP	A	263	19.066	43.197	53.431	1.00	29.73	AAAA
ATOM	2095	O	ASP	A	263	18.258	42.510	54.043	1.00	29.15	AAAA
ATOM	2096	N	TYR	A	264	19.002	43.416	52.122	1.00	31.25	AAAA
ATOM	2097	CA	TYR	A	264	17.925	42.888	51.306	1.00	32.43	AAAA
ATOM	2098	CB	TYR	A	264	17.913	43.558	49.938	1.00	34.53	AAAA
ATOM	2099	CG	TYR	A	264	17.627	45.038	49.997	1.00	38.21	AAAA
ATOM	2100	CD1	TYR	A	264	18.664	45.968	49.983	1.00	39.87	AAAA
ATOM	2101	CE1	TYR	A	264	18.409	47.335	50.068	1.00	41.74	AAAA
ATOM	2102	CD2	TYR	A	264	16.316	45.511	50.103	1.00	40.10	AAAA
ATOM	2103	CE2	TYR	A	264	16.044	46.877	50.191	1.00	41.50	AAAA
ATOM	2104	CZ	TYR	A	264	17.095	47.786	50.170	1.00	42.75	AAAA
ATOM	2105	OH	TYR	A	264	16.838	49.147	50.231	1.00	44.65	AAAA
ATOM	2106	C	TYR	A	264	17.897	41.385	51.135	1.00	32.50	AAAA
ATOM	2107	O	TYR	A	264	16.819	40.816	50.968	1.00	32.49	AAAA
ATOM	2108	N	LEU	A	265	19.064	40.740	51.171	1.00	32.64	AAAA
ATOM	2109	CA	LEU	A	265	19.122	39.281	51.036	1.00	31.92	AAAA
ATOM	2110	CB	LEU	A	265	20.525	38.823	50.617	1.00	32.75	AAAA
ATOM	2111	CG	LEU	A	265	20.808	39.010	49.127	1.00	32.95	AAAA
ATOM	2112	CD1	LEU	A	265	22.213	38.588	48.771	1.00	31.59	AAAA

Figure 19-33

ATOM	2113	CD2	LEU	A	265	19.803	38.166	48.361	1.00	34.62	AAAA
ATOM	2114	C	LEU	A	265	18.693	38.540	52.296	1.00	30.33	AAAA
ATOM	2115	O	LEU	A	265	19.024	37.375	52.484	1.00	30.30	AAAA
ATOM	2116	N	SER	A	266	17.945	39.230	53.147	1.00	29.23	AAAA
ATOM	2117	CA	SER	A	266	17.434	38.649	54.371	1.00	29.72	AAAA
ATOM	2118	CB	SER	A	266	18.398	38.894	55.519	1.00	32.09	AAAA
ATOM	2119	OG	SER	A	266	17.728	38.810	56.771	1.00	33.43	AAAA
ATOM	2120	C	SER	A	266	16.115	39.290	54.698	1.00	28.71	AAAA
ATOM	2121	O	SER	A	266	15.924	40.473	54.444	1.00	29.67	AAAA
ATOM	2122	N	LYS	A	267	15.209	38.517	55.276	1.00	27.82	AAAA
ATOM	2123	CA	LYS	A	267	13.908	39.045	55.654	1.00	27.56	AAAA
ATOM	2124	CB	LYS	A	267	12.821	38.076	55.222	1.00	28.75	AAAA
ATOM	2125	CG	LYS	A	267	12.733	37.922	53.718	1.00	29.67	AAAA
ATOM	2126	CD	LYS	A	267	12.343	39.223	53.053	1.00	30.13	AAAA
ATOM	2127	CE	LYS	A	267	12.303	39.036	51.546	1.00	31.86	AAAA
ATOM	2128	NZ	LYS	A	267	11.796	40.252	50.843	1.00	33.92	AAAA
ATOM	2129	C	LYS	A	267	13.800	39.327	57.152	1.00	27.18	AAAA
ATOM	2130	O	LYS	A	267	12.707	39.591	57.665	1.00	27.18	AAAA
ATOM	2131	N	PHE	A	268	14.944	39.267	57.836	1.00	26.12	AAAA
ATOM	2132	CA	PHE	A	268	15.048	39.532	59.271	1.00	25.72	AAAA
ATOM	2133	CB	PHE	A	268	16.272	38.830	59.856	1.00	24.94	AAAA
ATOM	2134	CG	PHE	A	268	16.167	37.334	59.896	1.00	25.07	AAAA
ATOM	2135	CD1	PHE	A	268	17.271	36.565	60.267	1.00	24.56	AAAA
ATOM	2136	CD2	PHE	A	268	14.955	36.687	59.629	1.00	23.76	AAAA
ATOM	2137	CE1	PHE	A	268	17.174	35.169	60.384	1.00	23.71	AAAA
ATOM	2138	CE2	PHE	A	268	14.850	35.303	59.739	1.00	23.86	AAAA
ATOM	2139	CZ	PHE	A	268	15.966	34.542	60.121	1.00	23.68	AAAA
ATOM	2140	C	PHE	A	268	15.190	41.030	59.513	1.00	25.77	AAAA
ATOM	2141	O	PHE	A	268	15.811	41.734	58.726	1.00	25.81	AAAA
ATOM	2142	N	ASN	A	269	14.606	41.524	60.595	1.00	26.02	AAAA
ATOM	2143	CA	ASN	A	269	14.718	42.943	60.890	1.00	26.58	AAAA
ATOM	2144	CB	ASN	A	269	13.330	43.584	61.058	1.00	25.47	AAAA
ATOM	2145	CG	ASN	A	269	12.379	43.252	59.906	1.00	25.37	AAAA
ATOM	2146	OD1	ASN	A	269	12.761	43.260	58.734	1.00	23.82	AAAA
ATOM	2147	ND2	ASN	A	269	11.123	42.985	60.245	1.00	24.03	AAAA
ATOM	2148	C	ASN	A	269	15.540	43.112	62.169	1.00	26.82	AAAA
ATOM	2149	O	ASN	A	269	15.089	43.715	63.150	1.00	27.98	AAAA
ATOM	2150	N	LEU	A	270	16.744	42.559	62.149	1.00	26.07	AAAA
ATOM	2151	CA	LEU	A	270	17.639	42.642	63.289	1.00	25.97	AAAA
ATOM	2152	CB	LEU	A	270	18.634	41.479	63.265	1.00	23.76	AAAA
ATOM	2153	CG	LEU	A	270	18.048	40.070	63.225	1.00	23.36	AAAA
ATOM	2154	CD1	LEU	A	270	19.115	39.090	63.710	1.00	21.90	AAAA
ATOM	2155	CD2	LEU	A	270	16.824	39.971	64.122	1.00	22.05	AAAA
ATOM	2156	C	LEU	A	270	18.420	43.961	63.360	1.00	27.13	AAAA
ATOM	2157	O	LEU	A	270	18.475	44.750	62.399	1.00	25.99	AAAA
ATOM	2158	N	SER	A	271	19.038	44.176	64.517	1.00	27.97	AAAA
ATOM	2159	CA	SER	A	271	19.832	45.370	64.767	1.00	27.95	AAAA
ATOM	2160	CB	SER	A	271	19.235	46.137	65.943	1.00	27.32	AAAA
ATOM	2161	OG	SER	A	271	19.184	45.297	67.089	1.00	27.90	AAAA
ATOM	2162	C	SER	A	271	21.276	44.987	65.084	1.00	28.15	AAAA
ATOM	2163	O	SER	A	271	21.574	43.832	65.401	1.00	26.99	AAAA
ATOM	2164	N	ASN	A	272	22.156	45.980	64.979	1.00	28.96	AAAA
ATOM	2165	CA	ASN	A	272	23.590	45.861	65.266	1.00	29.54	AAAA
ATOM	2166	CB	ASN	A	272	24.247	47.243	65.223	1.00	30.96	AAAA
ATOM	2167	CG	ASN	A	272	24.647	47.640	63.850	1.00	31.20	AAAA
ATOM	2168	OD1	ASN	A	272	24.960	48.794	63.594	1.00	31.73	AAAA
ATOM	2169	ND2	ASN	A	272	24.670	46.674	62.948	1.00	31.93	AAAA
ATOM	2170	C	ASN	A	272	23.821	45.309	66.645	1.00	29.63	AAAA
ATOM	2171	O	ASN	A	272	24.574	44.361	66.843	1.00	29.85	AAAA
ATOM	2172	N	VAL	A	273	23.180	45.959	67.600	1.00	29.77	AAAA
ATOM	2173	CA	VAL	A	273	23.290	45.602	68.994	1.00	30.89	AAAA
ATOM	2174	CB	VAL	A	273	22.436	46.576	69.816	1.00	31.61	AAAA
ATOM	2175	CG1	VAL	A	273	22.716	46.403	71.293	1.00	33.17	AAAA
ATOM	2176	CG2	VAL	A	273	22.740	47.998	69.372	1.00	31.82	AAAA
ATOM	2177	C	VAL	A	273	22.883	44.144	69.266	1.00	30.74	AAAA
ATOM	2178	O	VAL	A	273	23.550	43.431	70.022	1.00	31.23	AAAA

249/263 Figure 19-34

ATOM	2179	N	ALA	A	274	21.785	43.706	68.659	1.00	30.25	AAAA
ATOM	2180	CA	ALA	A	274	21.327	42.333	68.840	1.00	29.87	AAAA
ATOM	2181	CB	ALA	A	274	20.005	42.119	68.112	1.00	29.64	AAAA
ATOM	2182	C	ALA	A	274	22.395	41.438	68.247	1.00	29.35	AAAA
ATOM	2183	O	ALA	A	274	22.707	40.373	68.778	1.00	29.18	AAAA
ATOM	2184	N	PHE	A	275	22.946	41.893	67.127	1.00	29.30	AAAA
ATOM	2185	CA	PHE	A	275	23.991	41.170	66.428	1.00	28.91	AAAA
ATOM	2186	CB	PHE	A	275	24.375	41.909	65.150	1.00	28.77	AAAA
ATOM	2187	CG	PHE	A	275	25.354	41.170	64.308	1.00	28.08	AAAA
ATOM	2188	CD1	PHE	A	275	25.015	39.954	63.740	1.00	28.92	AAAA
ATOM	2189	CD2	PHE	A	275	26.621	41.684	64.077	1.00	29.48	AAAA
ATOM	2190	CE1	PHE	A	275	25.928	39.259	62.945	1.00	29.20	AAAA
ATOM	2191	CE2	PHE	A	275	27.546	40.988	63.279	1.00	29.24	AAAA
ATOM	2192	CZ	PHE	A	275	27.193	39.779	62.716	1.00	28.30	AAAA
ATOM	2193	C	PHE	A	275	25.196	41.058	67.351	1.00	27.64	AAAA
ATOM	2194	O	PHE	A	275	25.728	39.975	67.558	1.00	28.65	AAAA
ATOM	2195	N	LEU	A	276	25.606	42.189	67.902	1.00	26.81	AAAA
ATOM	2196	CA	LEU	A	276	26.732	42.260	68.831	1.00	27.38	AAAA
ATOM	2197	CB	LEU	A	276	26.878	43.700	69.353	1.00	27.53	AAAA
ATOM	2198	CG	LEU	A	276	28.202	44.213	69.928	1.00	26.37	AAAA
ATOM	2199	CD1	LEU	A	276	27.923	45.488	70.721	1.00	25.71	AAAA
ATOM	2200	CD2	LEU	A	276	28.842	43.189	70.827	1.00	27.06	AAAA
ATOM	2201	C	LEU	A	276	26.486	41.317	70.021	1.00	26.49	AAAA
ATOM	2202	O	LEU	A	276	27.387	40.603	70.471	1.00	25.26	AAAA
ATOM	2203	N	LYS	A	277	25.257	41.322	70.524	1.00	27.46	AAAA
ATOM	2204	CA	LYS	A	277	24.894	40.468	71.642	1.00	28.63	AAAA
ATOM	2205	CB	LYS	A	277	23.542	40.862	72.223	1.00	30.63	AAAA
ATOM	2206	CG	LYS	A	277	23.590	42.029	73.153	1.00	33.14	AAAA
ATOM	2207	CD	LYS	A	277	22.599	41.791	74.268	1.00	34.94	AAAA
ATOM	2208	CE	LYS	A	277	22.964	40.519	75.029	1.00	36.17	AAAA
ATOM	2209	NZ	LYS	A	277	21.979	40.194	76.104	1.00	38.64	AAAA
ATOM	2210	C	LYS	A	277	24.846	38.997	71.297	1.00	28.53	AAAA
ATOM	2211	O	LYS	A	277	25.118	38.152	72.146	1.00	28.45	AAAA
ATOM	2212	N	ALA	A	278	24.466	38.681	70.064	1.00	28.47	AAAA
ATOM	2213	CA	ALA	A	278	24.404	37.280	69.656	1.00	27.66	AAAA
ATOM	2214	CB	ALA	A	278	23.941	37.181	68.201	1.00	26.40	AAAA
ATOM	2215	C	ALA	A	278	25.833	36.754	69.820	1.00	26.63	AAAA
ATOM	2216	O	ALA	A	278	26.081	35.644	70.317	1.00	25.19	AAAA
ATOM	2217	N	PHE	A	279	26.764	37.616	69.427	1.00	26.50	AAAA
ATOM	2218	CA	PHE	A	279	28.181	37.345	69.481	1.00	25.83	AAAA
ATOM	2219	CB	PHE	A	279	28.934	38.521	68.869	1.00	26.35	AAAA
ATOM	2220	CG	PHE	A	279	30.413	38.319	68.796	1.00	27.92	AAAA
ATOM	2221	CD1	PHE	A	279	30.949	37.256	68.072	1.00	28.58	AAAA
ATOM	2222	CD2	PHE	A	279	31.280	39.201	69.434	1.00	28.33	AAAA
ATOM	2223	CE1	PHE	A	279	32.330	37.078	67.983	1.00	28.22	AAAA
ATOM	2224	CE2	PHE	A	279	32.666	39.030	69.349	1.00	28.11	AAAA
ATOM	2225	CZ	PHE	A	279	33.185	37.968	68.622	1.00	28.21	AAAA
ATOM	2226	C	PHE	A	279	28.665	37.118	70.901	1.00	25.47	AAAA
ATOM	2227	O	PHE	A	279	29.284	36.091	71.202	1.00	24.32	AAAA
ATOM	2228	N	ASN	A	280	28.382	38.075	71.778	1.00	25.12	AAAA
ATOM	2229	CA	ASN	A	280	28.841	37.944	73.147	1.00	25.05	AAAA
ATOM	2230	CB	ASN	A	280	28.708	39.269	73.887	1.00	24.42	AAAA
ATOM	2231	CG	ASN	A	280	29.683	40.300	73.364	1.00	24.56	AAAA
ATOM	2232	OD1	ASN	A	280	30.841	39.980	73.080	1.00	23.24	AAAA
ATOM	2233	ND2	ASN	A	280	29.233	41.543	73.249	1.00	24.59	AAAA
ATOM	2234	C	ASN	A	280	28.213	36.814	73.925	1.00	24.79	AAAA
ATOM	2235	O	ASN	A	280	28.828	36.272	74.825	1.00	24.96	AAAA
ATOM	2236	N	ILE	A	281	26.998	36.444	73.565	1.00	24.87	AAAA
ATOM	2237	CA	ILE	A	281	26.332	35.337	74.220	1.00	24.80	AAAA
ATOM	2238	CB	ILE	A	281	24.866	35.252	73.780	1.00	24.40	AAAA
ATOM	2239	CG2	ILE	A	281	24.297	33.907	74.124	1.00	25.03	AAAA
ATOM	2240	CD1	ILE	A	281	24.076	36.386	74.424	1.00	24.70	AAAA
ATOM	2241	C	ILE	A	281	22.613	36.379	74.069	1.00	26.49	AAAA
ATOM	2242	O	ILE	A	281	27.044	34.027	73.884	1.00	25.21	AAAA
ATOM	2243	N	VAL	A	282	27.220	33.170	74.750	1.00	24.97	AAAA
ATOM	2244	N	VAL	A	282	27.440	33.866	72.620	1.00	25.98	AAAA

Figure 19-35

ATOM	2245	CA	VAL	A	282	28.150	32.656	72.193	1.00	25.15	AAAA
ATOM	2246	CB	VAL	A	282	28.451	32.666	70.677	1.00	23.83	AAAA
ATOM	2247	CG1	VAL	A	282	29.315	31.470	70.311	1.00	23.58	AAAA
ATOM	2248	CG2	VAL	A	282	27.173	32.633	69.899	1.00	22.73	AAAA
ATOM	2249	C	VAL	A	282	29.478	32.553	72.936	1.00	25.73	AAAA
ATOM	2250	O	VAL	A	282	29.928	31.457	73.275	1.00	25.31	AAAA
ATOM	2251	N	ARG	A	283	30.100	33.702	73.176	1.00	26.90	AAAA
ATOM	2252	CA	ARG	A	283	31.372	33.760	73.885	1.00	28.87	AAAA
ATOM	2253	CB	ARG	A	283	32.027	35.131	73.684	1.00	28.16	AAAA
ATOM	2254	CG	ARG	A	283	32.364	35.440	72.240	1.00	27.22	AAAA
ATOM	2255	CD	ARG	A	283	32.821	36.862	72.098	1.00	27.08	AAAA
ATOM	2256	NE	ARG	A	283	34.035	37.116	72.854	1.00	26.73	AAAA
ATOM	2257	CZ	ARG	A	283	34.514	38.327	73.091	1.00	26.82	AAAA
ATOM	2258	NH1	ARG	A	283	33.873	39.384	72.626	1.00	27.36	AAAA
ATOM	2259	NH2	ARG	A	283	35.622	38.484	73.798	1.00	26.95	AAAA
ATOM	2260	C	ARG	A	283	31.183	33.494	75.376	1.00	30.71	AAAA
ATOM	2261	O	ARG	A	283	32.086	32.981	76.027	1.00	30.68	AAAA
ATOM	2262	N	GLU	A	284	30.014	33.842	75.911	1.00	32.71	AAAA
ATOM	2263	CA	GLU	A	284	29.735	33.623	77.323	1.00	35.53	AAAA
ATOM	2264	CB	GLU	A	284	28.482	34.391	77.751	1.00	37.39	AAAA
ATOM	2265	CG	GLU	A	284	28.538	35.854	77.392	1.00	41.73	AAAA
ATOM	2266	CD	GLU	A	284	27.272	36.631	77.754	1.00	45.27	AAAA
ATOM	2267	OE1	GLU	A	284	26.151	36.078	77.610	1.00	46.66	AAAA
ATOM	2268	OE2	GLU	A	284	27.405	37.817	78.148	1.00	46.94	AAAA
ATOM	2269	C	GLU	A	284	29.524	32.133	77.564	1.00	36.25	AAAA
ATOM	2270	O	GLU	A	284	29.920	31.593	78.601	1.00	37.85	AAAA
ATOM	2271	N	VAL	A	285	28.916	31.464	76.591	1.00	35.24	AAAA
ATOM	2272	CA	VAL	A	285	28.637	30.041	76.708	1.00	33.88	AAAA
ATOM	2273	CB	VAL	A	285	27.505	29.619	75.737	1.00	33.71	AAAA
ATOM	2274	CG1	VAL	A	285	27.201	28.137	75.888	1.00	32.59	AAAA
ATOM	2275	CG2	VAL	A	285	26.254	30.457	76.001	1.00	32.77	AAAA
ATOM	2276	C	VAL	A	285	29.847	29.149	76.456	1.00	33.47	AAAA
ATOM	2277	O	VAL	A	285	30.140	28.262	77.257	1.00	34.23	AAAA
ATOM	2278	N	PHE	A	286	30.568	29.389	75.364	1.00	32.34	AAAA
ATOM	2279	CA	PHE	A	286	31.706	28.535	75.036	1.00	29.92	AAAA
ATOM	2280	CB	PHE	A	286	31.533	27.960	73.635	1.00	29.77	AAAA
ATOM	2281	CG	PHE	A	286	30.267	27.179	73.444	1.00	28.64	AAAA
ATOM	2282	CD1	PHE	A	286	29.152	27.772	72.863	1.00	28.75	AAAA
ATOM	2283	CD2	PHE	A	286	30.197	25.837	73.827	1.00	28.55	AAAA
ATOM	2284	CE1	PHE	A	286	27.983	27.039	72.660	1.00	29.04	AAAA
ATOM	2285	CE2	PHE	A	286	29.037	25.095	73.629	1.00	28.19	AAAA
ATOM	2286	CZ	PHE	A	286	27.929	25.694	73.045	1.00	28.73	AAAA
ATOM	2287	C	PHE	A	286	33.106	29.113	75.132	1.00	29.13	AAAA
ATOM	2288	O	PHE	A	286	34.073	28.436	74.760	1.00	28.54	AAAA
ATOM	2289	N	GLY	A	287	33.224	30.341	75.637	1.00	28.42	AAAA
ATOM	2290	CA	GLY	A	287	34.525	30.987	75.744	1.00	27.07	AAAA
ATOM	2291	C	GLY	A	287	34.932	31.611	74.419	1.00	26.64	AAAA
ATOM	2292	O	GLY	A	287	34.088	32.042	73.649	1.00	27.13	AAAA
ATOM	2293	N	GLU	A	288	36.227	31.665	74.146	1.00	27.20	AAAA
ATOM	2294	CA	GLU	A	288	36.719	32.238	72.900	1.00	27.52	AAAA
ATOM	2295	CB	GLU	A	288	38.073	32.923	73.108	1.00	28.18	AAAA
ATOM	2296	CG	GLU	A	288	38.036	34.177	73.959	1.00	28.88	AAAA
ATOM	2297	CD	GLU	A	288	37.329	35.330	73.279	1.00	29.58	AAAA
ATOM	2298	OE1	GLU	A	288	37.807	35.813	72.243	1.00	29.94	AAAA
ATOM	2299	OE2	GLU	A	288	36.281	35.761	73.782	1.00	31.89	AAAA
ATOM	2300	C	GLU	A	288	36.877	31.158	71.843	1.00	27.44	AAAA
ATOM	2301	O	GLU	A	288	37.169	30.007	72.162	1.00	27.87	AAAA
ATOM	2302	N	GLY	A	289	36.663	31.547	70.589	1.00	26.55	AAAA
ATOM	2303	CA	GLY	A	289	36.795	30.638	69.466	1.00	25.25	AAAA
ATOM	2304	C	GLY	A	289	37.285	31.414	68.254	1.00	24.55	AAAA
ATOM	2305	O	GLY	A	289	37.635	32.586	68.369	1.00	24.40	AAAA
ATOM	2306	N	VAL	A	290	37.320	30.765	67.095	1.00	24.04	AAAA
ATOM	2307	CA	VAL	A	290	37.756	31.407	65.863	1.00	23.76	AAAA
ATOM	2308	CB	VAL	A	290	38.288	30.346	64.867	1.00	24.94	AAAA
ATOM	2309	CG1	VAL	A	290	38.835	31.012	63.596	1.00	22.73	AAAA
ATOM	2310	CG2	VAL	A	290	39.375	29.506	65.555	1.00	24.74	AAAA

ATOM	2311	C	VAL	A	290	36.536	32.122	65.277	1.00	23.90	AAAA
ATOM	2312	O	VAL	A	290	35.497	31.502	65.100	1.00	25.15	AAAA
ATOM	2313	N	TYR	A	291	36.662	33.415	64.976	1.00	23.09	AAAA
ATOM	2314	CA	TYR	A	291	35.544	34.211	64.446	1.00	21.41	AAAA
ATOM	2315	CB	TYR	A	291	35.472	35.540	65.193	1.00	20.57	AAAA
ATOM	2316	CG	TYR	A	291	35.511	35.346	66.677	1.00	19.87	AAAA
ATOM	2317	CD1	TYR	A	291	36.596	35.782	67.432	1.00	20.86	AAAA
ATOM	2318	CE1	TYR	A	291	36.677	35.513	68.793	1.00	21.47	AAAA
ATOM	2319	CD2	TYR	A	291	34.509	34.647	67.318	1.00	20.90	AAAA
ATOM	2320	CE2	TYR	A	291	34.579	34.372	68.675	1.00	21.90	AAAA
ATOM	2321	CZ	TYR	A	291	35.661	34.800	69.403	1.00	21.25	AAAA
ATOM	2322	OH	TYR	A	291	35.737	34.469	70.730	1.00	23.75	AAAA
ATOM	2323	C	TYR	A	291	35.607	34.483	62.946	1.00	21.25	AAAA
ATOM	2324	O	TYR	A	291	36.573	35.077	62.451	1.00	21.10	AAAA
ATOM	2325	N	LEU	A	292	34.557	34.084	62.231	1.00	20.92	AAAA
ATOM	2326	CA	LEU	A	292	34.518	34.260	60.779	1.00	20.92	AAAA
ATOM	2327	CB	LEU	A	292	34.235	32.916	60.080	1.00	19.93	AAAA
ATOM	2328	CG	LEU	A	292	35.104	31.688	60.399	1.00	17.31	AAAA
ATOM	2329	CD1	LEU	A	292	34.685	30.515	59.528	1.00	16.05	AAAA
ATOM	2330	CD2	LEU	A	292	36.552	32.000	60.163	1.00	18.07	AAAA
ATOM	2331	C	LEU	A	292	33.515	35.288	60.283	1.00	21.12	AAAA
ATOM	2332	O	LEU	A	292	32.652	35.741	61.020	1.00	20.70	AAAA
ATOM	2333	N	GLY	A	293	33.660	35.660	59.317	1.00	21.74	AAAA
ATOM	2334	CA	GLY	A	293	32.752	36.612	58.410	1.00	21.48	AAAA
ATOM	2335	C	GLY	A	293	31.612	35.856	57.770	1.00	21.65	AAAA
ATOM	2336	O	GLY	A	293	31.237	34.790	58.235	1.00	22.25	AAAA
ATOM	2337	N	GLY	A	294	31.060	36.392	56.691	1.00	22.66	AAAA
ATOM	2338	CA	GLY	A	294	29.957	35.714	56.034	1.00	23.61	AAAA
ATOM	2339	C	GLY	A	294	29.180	36.653	55.146	1.00	24.56	AAAA
ATOM	2340	O	GLY	A	294	29.679	37.727	54.790	1.00	25.54	AAAA
ATOM	2341	N	GLY	A	295	27.956	36.265	54.794	1.00	24.06	AAAA
ATOM	2342	CA	GLY	A	295	27.139	37.093	53.927	1.00	22.78	AAAA
ATOM	2343	C	GLY	A	295	26.902	38.479	54.483	1.00	23.11	AAAA
ATOM	2344	O	GLY	A	295	26.870	38.676	55.696	1.00	22.87	AAAA
ATOM	2345	N	GLY	A	296	26.733	39.442	53.584	1.00	22.78	AAAA
ATOM	2346	CA	GLY	A	296	26.497	40.813	53.993	1.00	23.44	AAAA
ATOM	2347	C	GLY	A	296	26.471	41.618	52.718	1.00	23.72	AAAA
ATOM	2348	O	GLY	A	296	27.474	41.661	52.004	1.00	23.73	AAAA
ATOM	2349	N	TYR	A	297	25.356	42.280	52.425	1.00	23.41	AAAA
ATOM	2350	CA	TYR	A	297	25.282	42.991	51.163	1.00	22.71	AAAA
ATOM	2351	CB	TYR	A	297	24.252	42.294	50.296	1.00	21.55	AAAA
ATOM	2352	CG	TYR	A	297	24.496	40.809	50.317	1.00	21.93	AAAA
ATOM	2353	CD1	TYR	A	297	24.036	40.016	51.375	1.00	20.95	AAAA
ATOM	2354	CE1	TYR	A	297	24.400	38.678	51.481	1.00	21.59	AAAA
ATOM	2355	CD2	TYR	A	297	25.320	40.217	49.358	1.00	21.71	AAAA
ATOM	2356	CE2	TYR	A	297	25.688	38.900	49.451	1.00	21.99	AAAA
ATOM	2357	CZ	TYR	A	297	25.242	38.127	50.511	1.00	22.18	AAAA
ATOM	2358	OH	TYR	A	297	25.721	36.841	50.615	1.00	21.35	AAAA
ATOM	2359	C	TYR	A	297	25.042	44.485	51.225	1.00	22.90	AAAA
ATOM	2360	O	TYR	A	297	25.106	45.172	50.203	1.00	23.17	AAAA
ATOM	2361	N	HIS	A	298	24.772	44.989	52.417	1.00	22.47	AAAA
ATOM	2362	CA	HIS	A	298	24.572	46.415	52.566	1.00	24.27	AAAA
ATOM	2363	CB	HIS	A	298	23.468	46.726	53.556	1.00	23.17	AAAA
ATOM	2364	CG	HIS	A	298	23.097	48.166	53.572	1.00	23.20	AAAA
ATOM	2365	CD2	HIS	A	298	23.588	49.201	54.287	1.00	24.25	AAAA
ATOM	2366	ND1	HIS	A	298	22.199	48.708	52.680	1.00	23.14	AAAA
ATOM	2367	CE1	HIS	A	298	22.151	50.017	52.848	1.00	23.31	AAAA
ATOM	2368	NE2	HIS	A	298	22.986	50.342	53.814	1.00	23.62	AAAA
ATOM	2369	C	HIS	A	298	25.886	46.976	53.106	1.00	25.17	AAAA
ATOM	2370	O	HIS	A	298	26.282	46.687	54.239	1.00	24.47	AAAA
ATOM	2371	N	PRO	A	299	26.563	47.818	52.316	1.00	26.37	AAAA
ATOM	2372	CD	PRO	A	299	26.178	48.372	51.006	1.00	27.01	AAAA
ATOM	2373	CA	PRO	A	299	27.840	48.394	52.752	1.00	27.31	AAAA
ATOM	2374	CB	PRO	A	299	28.156	49.383	51.630	1.00	27.04	AAAA
ATOM	2375	CG	PRO	A	299	26.743	49.764	51.120	1.00	27.57	AAAA
ATOM	2376	C	PRO	A	299	27.824	49.037	54.149	1.00	27.77	AAAA

ATOM	2377	O	PRO	A	299	28.755	48.826	54.939	1.00	28.04	AAAA
ATOM	2378	N	TYR	A	300	26.769	49.794	54.452	1.00	27.04	AAAA
ATOM	2379	CA	TYR	A	300	26.629	50.477	55.740	1.00	27.59	AAAA
ATOM	2380	CB	TYR	A	300	25.425	51.437	55.700	1.00	30.57	AAAA
ATOM	2381	CG	TYR	A	300	25.516	52.599	54.718	1.00	32.91	AAAA
ATOM	2382	CD1	TYR	A	300	26.181	52.464	53.491	1.00	33.45	AAAA
ATOM	2383	CE1	TYR	A	300	26.160	53.487	52.538	1.00	33.91	AAAA
ATOM	2384	CD2	TYR	A	300	24.837	53.801	54.969	1.00	34.19	AAAA
ATOM	2385	CE2	TYR	A	300	24.809	54.830	54.018	1.00	34.64	AAAA
ATOM	2386	CZ	TYR	A	300	25.468	54.657	52.807	1.00	34.56	AAAA
ATOM	2387	OH	TYR	A	300	25.389	55.630	51.844	1.00	36.05	AAAA
ATOM	2388	C	TYR	A	300	26.454	49.538	56.936	1.00	26.48	AAAA
ATOM	2389	O	TYR	A	300	27.073	49.726	57.979	1.00	25.81	AAAA
ATOM	2390	N	ALA	A	301	25.581	48.547	56.791	1.00	25.41	AAAA
ATOM	2391	CA	ALA	A	301	25.328	47.606	57.865	1.00	24.64	AAAA
ATOM	2392	CB	ALA	A	301	24.164	46.731	57.511	1.00	25.32	AAAA
ATOM	2393	C	ALA	A	301	26.568	46.775	58.067	1.00	25.53	AAAA
ATOM	2394	O	ALA	A	301	27.030	46.567	59.194	1.00	26.39	AAAA
ATOM	2395	N	LEU	A	302	27.108	46.304	56.950	1.00	25.83	AAAA
ATOM	2396	CA	LEU	A	302	28.323	45.500	56.926	1.00	26.32	AAAA
ATOM	2397	CB	LEU	A	302	28.782	45.378	55.479	1.00	27.38	AAAA
ATOM	2398	CG	LEU	A	302	30.081	44.723	55.024	1.00	28.18	AAAA
ATOM	2399	CD1	LEU	A	302	30.119	44.840	53.502	1.00	29.32	AAAA
ATOM	2400	CD2	LEU	A	302	31.296	45.389	55.613	1.00	27.38	AAAA
ATOM	2401	C	LEU	A	302	29.398	46.187	57.764	1.00	26.41	AAAA
ATOM	2402	O	LEU	A	302	29.874	45.648	58.755	1.00	26.62	AAAA
ATOM	2403	N	ALA	A	303	29.756	47.397	57.353	1.00	26.50	AAAA
ATOM	2404	CA	ALA	A	303	30.778	48.176	58.022	1.00	25.92	AAAA
ATOM	2405	CB	ALA	A	303	31.001	49.475	57.277	1.00	25.24	AAAA
ATOM	2406	C	ALA	A	303	30.490	48.464	59.487	1.00	26.03	AAAA
ATOM	2407	O	ALA	A	303	31.325	48.175	60.340	1.00	26.95	AAAA
ATOM	2408	N	ARG	A	304	29.322	49.028	59.792	1.00	25.29	AAAA
ATOM	2409	CA	ARG	A	304	28.999	49.353	61.179	1.00	23.46	AAAA
ATOM	2410	CB	ARG	A	304	27.641	50.059	61.291	1.00	23.78	AAAA
ATOM	2411	CG	ARG	A	304	27.553	51.451	60.629	1.00	24.59	AAAA
ATOM	2412	CD	ARG	A	304	26.302	52.223	61.091	1.00	25.85	AAAA
ATOM	2413	NE	ARG	A	304	25.067	51.465	60.869	1.00	27.54	AAAA
ATOM	2414	CZ	ARG	A	304	23.978	51.547	61.637	1.00	28.36	AAAA
ATOM	2415	NH1	ARG	A	304	23.957	52.362	62.695	1.00	26.48	AAAA
ATOM	2416	NH2	ARG	A	304	22.910	50.794	61.358	1.00	28.45	AAAA
ATOM	2417	C	ARG	A	304	28.991	48.118	62.053	1.00	23.18	AAAA
ATOM	2418	O	ARG	A	304	29.591	48.099	63.135	1.00	22.26	AAAA
ATOM	2419	N	ALA	A	305	28.330	47.075	61.560	1.00	23.20	AAAA
ATOM	2420	CA	ALA	A	305	28.200	45.817	62.292	1.00	22.33	AAAA
ATOM	2421	CB	ALA	A	305	27.319	44.866	61.516	1.00	22.17	AAAA
ATOM	2422	C	ALA	A	305	29.516	45.137	62.621	1.00	22.27	AAAA
ATOM	2423	O	ALA	A	305	29.763	44.757	63.760	1.00	22.48	AAAA
ATOM	2424	N	TRP	A	306	30.366	44.969	61.620	1.00	22.57	AAAA
ATOM	2425	CA	TRP	A	306	31.634	44.307	61.861	1.00	21.28	AAAA
ATOM	2426	CB	TRP	A	306	32.279	43.885	60.553	1.00	21.07	AAAA
ATOM	2427	CG	TRP	A	306	31.703	42.618	60.004	1.00	20.75	AAAA
ATOM	2428	CD2	TRP	A	306	31.886	42.103	58.683	1.00	19.54	AAAA
ATOM	2429	CE2	TRP	A	306	31.352	40.795	58.668	1.00	19.18	AAAA
ATOM	2430	CE3	TRP	A	306	32.456	42.616	57.510	1.00	19.59	AAAA
ATOM	2431	CD1	TRP	A	306	31.071	41.632	60.713	1.00	20.51	AAAA
ATOM	2432	NE1	TRP	A	306	30.864	40.537	59.922	1.00	19.74	AAAA
ATOM	2433	CZ2	TRP	A	306	31.368	39.990	57.524	1.00	19.18	AAAA
ATOM	2434	CZ3	TRP	A	306	32.474	41.810	56.367	1.00	18.98	AAAA
ATOM	2435	CH2	TRP	A	306	31.933	40.513	56.388	1.00	19.21	AAAA
ATOM	2436	C	TRP	A	306	32.571	45.159	62.674	1.00	20.80	AAAA
ATOM	2437	O	TRP	A	306	33.459	44.630	63.341	1.00	20.55	AAAA
ATOM	2438	N	THR	A	307	32.373	46.475	62.614	1.00	20.17	AAAA
ATOM	2439	CA	THR	A	307	33.175	47.399	63.407	1.00	20.54	AAAA
ATOM	2440	CB	THR	A	307	32.861	48.881	63.045	1.00	21.09	AAAA
ATOM	2441	OG1	THR	A	307	33.329	49.159	61.718	1.00	21.25	AAAA
ATOM	2442	CG2	THR	A	307	33.523	49.839	64.030	1.00	20.09	AAAA

253/263 Figure 19-38

ATOM	2443	C	THR	A	307	32.853	47.135	64.893	1.00	20.88	AAAA
ATOM	2444	O	THR	A	307	33.738	47.175	65.747	1.00	21.89	AAAA
ATOM	2445	N	LEU	A	308	31.588	46.851	65.192	1.00	20.10	AAAA
ATOM	2446	CA	LEU	A	308	31.189	46.543	66.559	1.00	21.10	AAAA
ATOM	2447	CB	LEU	A	308	29.671	46.340	66.644	1.00	20.99	AAAA
ATOM	2448	CG	LEU	A	308	28.897	47.656	66.674	1.00	21.54	AAAA
ATOM	2449	CD1	LEU	A	308	27.397	47.473	66.411	1.00	19.91	AAAA
ATOM	2450	CD2	LEU	A	308	29.177	48.283	68.045	1.00	21.04	AAAA
ATOM	2451	C	LEU	A	308	31.886	45.284	67.052	1.00	21.98	AAAA
ATOM	2452	O	LEU	A	308	32.284	45.186	68.215	1.00	22.17	AAAA
ATOM	2453	N	ILE	A	309	32.023	44.310	66.165	1.00	22.32	AAAA
ATOM	2454	CA	ILE	A	309	32.658	43.069	66.544	1.00	23.12	AAAA
ATOM	2455	CB	ILE	A	309	32.590	42.016	65.413	1.00	22.33	AAAA
ATOM	2456	CG2	ILE	A	309	33.356	40.787	65.827	1.00	21.76	AAAA
ATOM	2457	CG1	ILE	A	309	31.140	41.678	65.061	1.00	22.16	AAAA
ATOM	2458	CD1	ILE	A	309	30.366	41.037	66.166	1.00	22.01	AAAA
ATOM	2459	C	ILE	A	309	34.115	43.377	66.790	1.00	24.52	AAAA
ATOM	2460	O	ILE	A	309	34.734	42.828	67.709	1.00	25.72	AAAA
ATOM	2461	N	TRP	A	310	34.673	44.253	65.957	1.00	24.70	AAAA
ATOM	2462	CA	TRP	A	310	36.075	44.570	66.099	1.00	24.20	AAAA
ATOM	2463	CB	TRP	A	310	36.587	45.417	64.944	1.00	23.29	AAAA
ATOM	2464	CG	TRP	A	310	38.040	45.712	65.123	1.00	23.17	AAAA
ATOM	2465	CD2	TRP	A	310	39.104	44.752	65.257	1.00	21.36	AAAA
ATOM	2466	CE2	TRP	A	310	40.291	45.472	65.490	1.00	20.62	AAAA
ATOM	2467	CE3	TRP	A	310	39.165	43.354	65.202	1.00	20.01	AAAA
ATOM	2468	CD1	TRP	A	310	38.614	46.938	65.273	1.00	22.82	AAAA
ATOM	2469	NE1	TRP	A	310	39.967	46.803	65.497	1.00	22.30	AAAA
ATOM	2470	CZ2	TRP	A	310	41.521	44.845	65.668	1.00	19.91	AAAA
ATOM	2471	CZ3	TRP	A	310	40.388	42.734	65.381	1.00	19.08	AAAA
ATOM	2472	CH2	TRP	A	310	41.547	43.477	65.610	1.00	19.40	AAAA
ATOM	2473	C	TRP	A	310	36.318	45.279	67.411	1.00	25.26	AAAA
ATOM	2474	O	TRP	A	310	37.262	44.945	68.109	1.00	24.71	AAAA
ATOM	2475	N	CYS	A	311	35.467	46.247	67.749	1.00	26.76	AAAA
ATOM	2476	CA	CYS	A	311	35.608	46.975	69.007	1.00	27.89	AAAA
ATOM	2477	CB	CYS	A	311	34.548	48.081	69.113	1.00	28.98	AAAA
ATOM	2478	SG	CYS	A	311	34.798	49.462	67.991	1.00	31.89	AAAA
ATOM	2479	C	CYS	A	311	35.495	46.043	70.212	1.00	27.51	AAAA
ATOM	2480	O	CYS	A	311	36.289	46.127	71.135	1.00	26.90	AAAA
ATOM	2481	N	GLU	A	312	34.495	45.169	70.187	1.00	27.33	AAAA
ATOM	2482	CA	GLU	A	312	34.246	44.210	71.250	1.00	28.03	AAAA
ATOM	2483	CB	GLU	A	312	33.106	43.287	70.850	1.00	28.55	AAAA
ATOM	2484	CG	GLU	A	312	31.903	43.333	71.741	1.00	28.93	AAAA
ATOM	2485	CD	GLU	A	312	32.232	42.958	73.154	1.00	29.78	AAAA
ATOM	2486	OE1	GLU	A	312	32.954	41.957	73.345	1.00	30.81	AAAA
ATOM	2487	OE2	GLU	A	312	31.754	43.653	74.071	1.00	30.79	AAAA
ATOM	2488	C	GLU	A	312	35.463	43.357	71.514	1.00	28.91	AAAA
ATOM	2489	O	GLU	A	312	35.822	43.110	72.662	1.00	30.57	AAAA
ATOM	2490	N	LEU	A	313	36.081	42.889	70.436	1.00	29.04	AAAA
ATOM	2491	CA	LEU	A	313	37.266	42.045	70.516	1.00	28.87	AAAA
ATOM	2492	CB	LEU	A	313	37.524	41.373	69.157	1.00	29.39	AAAA
ATOM	2493	CG	LEU	A	313	36.548	40.311	68.644	1.00	30.32	AAAA
ATOM	2494	CD1	LEU	A	313	36.910	39.872	67.215	1.00	30.26	AAAA
ATOM	2495	CD2	LEU	A	313	36.582	39.114	69.593	1.00	30.42	AAAA
ATOM	2496	C	LEU	A	313	38.474	42.888	70.905	1.00	27.75	AAAA
ATOM	2497	O	LEU	A	313	39.215	42.553	71.808	1.00	27.34	AAAA
ATOM	2498	N	SER	A	314	38.642	43.986	70.191	1.00	27.95	AAAA
ATOM	2499	CA	SER	A	314	39.736	44.927	70.376	1.00	28.62	AAAA
ATOM	2500	CB	SER	A	314	39.690	45.937	69.231	1.00	27.49	AAAA
ATOM	2501	OG	SER	A	314	40.703	46.904	69.343	1.00	30.12	AAAA
ATOM	2502	C	SER	A	314	39.666	45.653	71.727	1.00	29.67	AAAA
ATOM	2503	O	SER	A	314	40.488	46.517	72.023	1.00	29.00	AAAA
ATOM	2504	N	GLY	A	315	38.676	45.302	72.538	1.00	30.78	AAAA
ATOM	2505	CA	GLY	A	315	38.535	45.935	73.827	1.00	32.92	AAAA
ATOM	2506	C	GLY	A	315	38.542	47.452	73.784	1.00	34.92	AAAA
ATOM	2507	O	GLY	A	315	39.142	48.091	74.647	1.00	35.17	AAAA
ATOM	2508	N	ARG	A	316	37.881	48.041	72.794	1.00	36.88	AAAA

ATOM	2509	CA	ARG	A	316	37.841	49.493	72.702	1.00	39.49	AAAA
ATOM	2510	CB	ARG	A	316	38.608	49.968	71.484	1.00	39.86	AAAA
ATOM	2511	CG	ARG	A	316	37.946	49.677	70.161	1.00	40.77	AAAA
ATOM	2512	CD	ARG	A	316	38.843	50.226	69.077	1.00	41.47	AAAA
ATOM	2513	NE	ARG	A	316	40.140	49.566	69.092	1.00	42.36	AAAA
ATOM	2514	CZ	ARG	A	316	41.224	50.057	68.515	1.00	43.38	AAAA
ATOM	2515	NH1	ARG	A	316	41.159	51.217	67.882	1.00	44.76	AAAA
ATOM	2516	NH2	ARG	A	316	42.361	49.385	68.556	1.00	43.71	AAAA
ATOM	2517	C	ARG	A	316	36.418	50.015	72.631	1.00	41.54	AAAA
ATOM	2518	O	ARG	A	316	35.564	49.429	71.959	1.00	42.64	AAAA
ATOM	2519	N	GLU	A	317	36.163	51.119	73.329	1.00	43.10	AAAA
ATOM	2520	CA	GLU	A	317	34.830	51.720	73.356	1.00	44.51	AAAA
ATOM	2521	CB	GLU	A	317	34.809	52.936	74.293	1.00	46.17	AAAA
ATOM	2522	CG	GLU	A	317	34.472	52.614	75.759	1.00	49.65	AAAA
ATOM	2523	CD	GLU	A	317	35.426	51.623	76.439	1.00	52.51	AAAA
ATOM	2524	OE1	GLU	A	317	35.153	51.251	77.607	1.00	53.37	AAAA
ATOM	2525	OE2	GLU	A	317	36.444	51.214	75.831	1.00	54.14	AAAA
ATOM	2526	C	GLU	A	317	34.318	52.098	71.974	1.00	43.86	AAAA
ATOM	2527	O	GLU	A	317	35.067	52.532	71.108	1.00	42.46	AAAA
ATOM	2528	N	VAL	A	318	33.023	51.916	71.779	1.00	44.79	AAAA
ATOM	2529	CA	VAL	A	318	32.394	52.197	70.502	1.00	45.57	AAAA
ATOM	2530	CB	VAL	A	318	31.098	51.369	70.324	1.00	45.36	AAAA
ATOM	2531	CG1	VAL	A	318	30.537	51.558	68.924	1.00	45.44	AAAA
ATOM	2532	CG2	VAL	A	318	31.366	49.911	70.612	1.00	46.35	AAAA
ATOM	2533	C	VAL	A	318	32.007	53.652	70.377	1.00	46.41	AAAA
ATOM	2534	O	VAL	A	318	31.199	54.145	71.165	1.00	46.53	AAAA
ATOM	2535	N	PRO	A	319	32.584	54.370	69.396	1.00	46.89	AAAA
ATOM	2536	CD	PRO	A	319	33.581	54.017	68.375	1.00	46.44	AAAA
ATOM	2537	CA	PRO	A	319	32.209	55.774	69.247	1.00	47.62	AAAA
ATOM	2538	CB	PRO	A	319	33.022	56.206	68.024	1.00	46.96	AAAA
ATOM	2539	CG	PRO	A	319	33.161	54.922	67.251	1.00	46.38	AAAA
ATOM	2540	C	PRO	A	319	30.709	55.743	68.977	1.00	48.64	AAAA
ATOM	2541	O	PRO	A	319	30.236	54.860	68.262	1.00	48.61	AAAA
ATOM	2542	N	GLU	A	320	29.944	56.667	69.544	1.00	49.24	AAAA
ATOM	2543	CA	GLU	A	320	28.522	56.598	69.288	1.00	50.01	AAAA
ATOM	2544	CB	GLU	A	320	27.720	57.330	70.363	1.00	51.15	AAAA
ATOM	2545	CG	GLU	A	320	27.828	58.831	70.339	1.00	53.01	AAAA
ATOM	2546	CD	GLU	A	320	26.825	59.474	71.282	1.00	54.34	AAAA
ATOM	2547	OE1	GLU	A	320	25.604	59.273	71.077	1.00	54.04	AAAA
ATOM	2548	OE2	GLU	A	320	27.255	60.171	72.228	1.00	55.06	AAAA
ATOM	2549	C	GLU	A	320	28.206	57.168	67.921	1.00	49.78	AAAA
ATOM	2550	O	GLU	A	320	27.170	56.861	67.324	1.00	49.79	AAAA
ATOM	2551	N	LYS	A	321	29.116	57.980	67.407	1.00	49.26	AAAA
ATOM	2552	CA	LYS	A	321	28.906	58.589	66.109	1.00	49.20	AAAA
ATOM	2553	CB	LYS	A	321	28.873	60.106	66.251	1.00	50.38	AAAA
ATOM	2554	CG	LYS	A	321	30.234	60.674	66.634	1.00	52.88	AAAA
ATOM	2555	CD	LYS	A	321	30.717	60.180	68.002	1.00	53.76	AAAA
ATOM	2556	CE	LYS	A	321	32.229	60.348	68.154	1.00	55.00	AAAA
ATOM	2557	NZ	LYS	A	321	32.715	61.725	67.829	1.00	55.95	AAAA
ATOM	2558	C	LYS	A	321	30.037	58.207	65.171	1.00	48.64	AAAA
ATOM	2559	O	LYS	A	321	31.052	57.650	65.590	1.00	48.58	AAAA
ATOM	2560	N	LEU	A	322	29.854	58.511	63.894	1.00	47.78	AAAA
ATOM	2561	CA	LEU	A	322	30.870	58.238	62.896	1.00	46.13	AAAA
ATOM	2562	CB	LEU	A	322	30.248	57.638	61.638	1.00	46.84	AAAA
ATOM	2563	CG	LEU	A	322	29.240	56.504	61.848	1.00	47.71	AAAA
ATOM	2564	CD1	LEU	A	322	28.788	55.998	60.491	1.00	48.02	AAAA
ATOM	2565	CD2	LEU	A	322	29.853	55.374	62.667	1.00	48.21	AAAA
ATOM	2566	C	LEU	A	322	31.427	59.608	62.580	1.00	44.61	AAAA
ATOM	2567	O	LEU	A	322	30.674	60.571	62.491	1.00	44.73	AAAA
ATOM	2568	N	ASN	A	323	32.741	59.706	62.447	1.00	42.66	AAAA
ATOM	2569	CA	ASN	A	323	33.360	60.976	62.135	1.00	41.19	AAAA
ATOM	2570	CB	ASN	A	323	34.860	60.904	62.402	1.00	41.07	AAAA
ATOM	2571	CG	ASN	A	323	35.576	60.001	61.436	1.00	41.43	AAAA
ATOM	2572	OD1	ASN	A	323	35.117	58.901	61.147	1.00	42.46	AAAA
ATOM	2573	ND2	ASN	A	323	36.720	60.449	60.943	1.00	41.77	AAAA
ATOM	2574	C	ASN	A	323	33.068	61.223	60.658	1.00	40.76	AAAA

255/263 Figure 19-40

ATOM	2575	O	ASN A 323	32.430	60.395	60.010	1.00	40.19	AAAA
ATOM	2576	N	ASN A 324	33.523	62.352	60.129	1.00	40.11	AAAA
ATOM	2577	CA	ASN A 324	33.268	62.699	58.735	1.00	39.99	AAAA
ATOM	2578	CB	ASN A 324	33.711	64.128	58.472	1.00	39.54	AAAA
ATOM	2579	CG	ASN A 324	33.003	65.114	59.361	1.00	40.88	AAAA
ATOM	2580	OD1	ASN A 324	31.763	65.145	59.417	1.00	40.77	AAAA
ATOM	2581	ND2	ASN A 324	33.779	65.938	60.064	1.00	40.63	AAAA
ATOM	2582	C	ASN A 324	33.918	61.786	57.712	1.00	40.10	AAAA
ATOM	2583	O	ASN A 324	33.320	61.468	56.678	1.00	39.24	AAAA
ATOM	2584	N	LYS A 325	35.144	61.376	58.011	1.00	40.41	AAAA
ATOM	2585	CA	LYS A 325	35.908	60.519	57.126	1.00	41.41	AAAA
ATOM	2586	CB	LYS A 325	37.262	60.201	57.761	1.00	42.64	AAAA
ATOM	2587	CG	LYS A 325	38.224	59.504	56.828	1.00	44.45	AAAA
ATOM	2588	CD	LYS A 325	39.575	59.199	57.491	1.00	45.61	AAAA
ATOM	2589	CE	LYS A 325	40.358	60.464	57.850	1.00	45.88	AAAA
ATOM	2590	NZ	LYS A 325	41.717	60.151	58.404	1.00	46.27	AAAA
ATOM	2591	C	LYS A 325	35.124	59.248	56.856	1.00	41.56	AAAA
ATOM	2592	O	LYS A 325	35.042	58.781	55.716	1.00	41.35	AAAA
ATOM	2593	N	ALA A 326	34.524	58.703	57.906	1.00	41.32	AAAA
ATOM	2594	CA	ALA A 326	33.732	57.492	57.774	1.00	41.07	AAAA
ATOM	2595	CB	ALA A 326	33.452	56.912	59.143	1.00	40.87	AAAA
ATOM	2596	C	ALA A 326	32.420	57.722	57.019	1.00	41.24	AAAA
ATOM	2597	O	ALA A 326	32.045	56.913	56.174	1.00	40.91	AAAA
ATOM	2598	N	LYS A 327	31.719	58.815	57.316	1.00	41.92	AAAA
ATOM	2599	CA	LYS A 327	30.451	59.097	56.631	1.00	42.20	AAAA
ATOM	2600	CB	LYS A 327	29.796	60.374	57.170	1.00	43.61	AAAA
ATOM	2601	CG	LYS A 327	29.534	60.413	58.670	1.00	45.83	AAAA
ATOM	2602	CD	LYS A 327	28.745	61.681	59.029	1.00	47.34	AAAA
ATOM	2603	CE	LYS A 327	28.682	61.952	60.538	1.00	48.28	AAAA
ATOM	2604	NZ	LYS A 327	28.090	60.845	61.351	1.00	48.98	AAAA
ATOM	2605	C	LYS A 327	30.673	59.266	55.125	1.00	41.33	AAAA
ATOM	2606	O	LYS A 327	29.879	58.797	54.309	1.00	40.78	AAAA
ATOM	2607	N	GLU A 328	31.761	59.950	54.781	1.00	40.39	AAAA
ATOM	2608	CA	GLU A 328	32.129	60.217	53.399	1.00	38.91	AAAA
ATOM	2609	CB	GLU A 328	33.300	61.199	53.369	1.00	40.04	AAAA
ATOM	2610	CG	GLU A 328	32.941	62.576	53.909	1.00	41.94	AAAA
ATOM	2611	CD	GLU A 328	34.131	63.515	53.994	1.00	43.77	AAAA
ATOM	2612	OE1	GLU A 328	34.904	63.595	53.010	1.00	44.29	AAAA
ATOM	2613	OE2	GLU A 328	34.285	64.189	55.040	1.00	45.11	AAAA
ATOM	2614	C	GLU A 328	32.497	58.938	52.675	1.00	37.39	AAAA
ATOM	2615	O	GLU A 328	32.114	58.722	51.525	1.00	37.31	AAAA
ATOM	2616	N	LEU A 329	33.255	58.091	53.355	1.00	35.67	AAAA
ATOM	2617	CA	LEU A 329	33.657	56.820	52.783	1.00	33.03	AAAA
ATOM	2618	CB	LEU A 329	34.451	56.012	53.813	1.00	30.62	AAAA
ATOM	2619	CG	LEU A 329	34.760	54.549	53.481	1.00	27.48	AAAA
ATOM	2620	CD1	LEU A 329	35.549	54.453	52.193	1.00	26.24	AAAA
ATOM	2621	CD2	LEU A 329	35.514	53.936	54.622	1.00	25.74	AAAA
ATOM	2622	C	LEU A 329	32.405	56.057	52.368	1.00	23.24	AAAA
ATOM	2623	O	LEU A 329	32.239	55.708	51.205	1.00	32.72	AAAA
ATOM	2624	N	LEU A 330	31.519	55.810	53.327	1.00	33.92	AAAA
ATOM	2625	CA	LEU A 330	30.289	55.090	53.046	1.00	34.91	AAAA
ATOM	2626	CB	LEU A 330	29.411	55.023	54.292	1.00	34.02	AAAA
ATOM	2627	CG	LEU A 330	30.067	54.236	55.418	1.00	34.06	AAAA
ATOM	2628	CD1	LEU A 330	29.096	54.060	56.571	1.00	33.63	AAAA
ATOM	2629	CD2	LEU A 330	30.512	52.892	54.884	1.00	33.82	AAAA
ATOM	2630	C	LEU A 330	29.499	55.695	51.907	1.00	35.94	AAAA
ATOM	2631	O	LEU A 330	28.984	54.968	51.060	1.00	36.14	AAAA
ATOM	2632	N	LYS A 331	29.415	57.022	51.883	1.00	38.17	AAAA
ATOM	2633	CA	LYS A 331	28.664	57.718	50.845	1.00	41.05	AAAA
ATOM	2634	CB	LYS A 331	28.407	59.161	51.233	1.00	41.83	AAAA
ATOM	2635	CG	LYS A 331	27.584	59.358	52.497	1.00	43.26	AAAA
ATOM	2636	CD	LYS A 331	27.202	60.823	52.755	1.00	44.15	AAAA
ATOM	2637	CE	LYS A 331	26.182	61.333	51.730	1.00	45.71	AAAA
ATOM	2638	NZ	LYS A 331	25.695	62.735	51.993	1.00	45.95	AAAA
ATOM	2639	C	LYS A 331	29.342	57.581	49.490	1.00	42.22	AAAA
ATOM	2640	O	LYS A 331	28.712	57.980	48.480	1.00	41.94	AAAA

256/263 Figure 19-41

ATOM	2641	N	SER	A	332	30.618	57.316	49.463	1.00	44.45	AAAA
ATOM	2642	CA	SER	A	332	31.351	57.271	48.202	1.00	46.88	AAAA
ATOM	2643	CB	SER	A	332	32.854	57.416	48.435	1.00	46.49	AAAA
ATOM	2644	OG	SER	A	332	33.380	56.263	49.058	1.00	45.65	AAAA
ATOM	2645	C	SER	A	332	31.093	55.959	47.494	1.00	48.73	AAAA
ATOM	2646	O	SER	A	332	31.262	55.854	46.281	1.00	49.51	AAAA
ATOM	2647	N	ILE	A	333	30.697	54.952	48.258	1.00	50.62	AAAA
ATOM	2648	CA	ILE	A	333	30.420	53.648	47.686	1.00	52.65	AAAA
ATOM	2649	CB	ILE	A	333	30.246	52.584	48.779	1.00	52.35	AAAA
ATOM	2650	CG2	ILE	A	333	29.889	51.248	48.157	1.00	51.40	AAAA
ATOM	2651	CG1	ILE	A	333	31.522	52.465	49.596	1.00	52.29	AAAA
ATOM	2652	CD1	ILE	A	333	31.403	51.463	50.696	1.00	53.23	AAAA
ATOM	2653	C	ILE	A	333	29.120	53.712	46.924	1.00	54.42	AAAA
ATOM	2654	O	ILE	A	333	28.122	54.178	47.462	1.00	55.10	AAAA
ATOM	2655	N	ASP	A	334	29.118	53.274	45.672	1.00	56.56	AAAA
ATOM	2656	CA	ASP	A	334	27.863	53.263	44.940	1.00	59.13	AAAA
ATOM	2657	CB	ASP	A	334	28.050	53.460	43.433	1.00	59.64	AAAA
ATOM	2658	CG	ASP	A	334	28.976	52.446	42.823	1.00	59.23	AAAA
ATOM	2659	OD1	ASP	A	334	28.853	52.194	41.606	1.00	58.87	AAAA
ATOM	2660	OD2	ASP	A	334	29.839	51.925	43.559	1.00	59.34	AAAA
ATOM	2661	C	ASP	A	334	27.251	51.898	45.215	1.00	60.95	AAAA
ATOM	2662	O	ASP	A	334	27.803	50.861	44.840	1.00	61.15	AAAA
ATOM	2663	N	PHE	A	335	26.113	51.914	45.897	1.00	62.56	AAAA
ATOM	2664	CA	PHE	A	335	25.414	50.701	46.257	1.00	64.12	AAAA
ATOM	2665	CB	PHE	A	335	25.311	50.621	47.779	1.00	64.40	AAAA
ATOM	2666	CG	PHE	A	335	24.224	49.714	48.263	1.00	64.98	AAAA
ATOM	2667	CD1	PHE	A	335	24.180	48.379	47.868	1.00	65.54	AAAA
ATOM	2668	CD2	PHE	A	335	23.234	50.197	49.107	1.00	65.12	AAAA
ATOM	2669	CE1	PHE	A	335	23.163	47.539	48.305	1.00	65.75	AAAA
ATOM	2670	CE2	PHE	A	335	22.213	49.367	49.552	1.00	65.79	AAAA
ATOM	2671	CZ	PHE	A	335	22.177	48.034	49.150	1.00	66.01	AAAA
ATOM	2672	C	PHE	A	335	24.025	50.626	45.640	1.00	65.41	AAAA
ATOM	2673	O	PHE	A	335	23.591	49.564	45.184	1.00	65.27	AAAA
ATOM	2674	N	GLU	A	336	23.338	51.763	45.618	1.00	66.38	AAAA
ATOM	2675	CA	GLU	A	336	21.980	51.826	45.097	1.00	67.49	AAAA
ATOM	2676	CB	GLU	A	336	21.893	51.260	43.673	1.00	68.25	AAAA
ATOM	2677	CG	GLU	A	336	20.459	51.230	43.116	1.00	69.15	AAAA
ATOM	2678	CD	GLU	A	336	20.334	50.465	41.804	1.00	69.40	AAAA
ATOM	2679	OE1	GLU	A	336	20.710	49.271	41.784	1.00	69.57	AAAA
ATOM	2680	OE2	GLU	A	336	19.851	51.051	40.804	1.00	69.10	AAAA
ATOM	2681	C	GLU	A	336	21.098	50.999	46.025	1.00	67.68	AAAA
ATOM	2682	O	GLU	A	336	21.216	49.776	46.082	1.00	67.58	AAAA
ATOM	2683	N	GLU	A	337	20.227	51.679	46.761	1.00	67.87	AAAA
ATOM	2684	CA	GLU	A	337	19.317	51.020	47.686	1.00	68.66	AAAA
ATOM	2685	CB	GLU	A	337	18.583	52.085	48.502	1.00	68.88	AAAA
ATOM	2686	CG	GLU	A	337	18.279	51.715	49.944	1.00	68.12	AAAA
ATOM	2687	CD	GLU	A	337	19.527	51.587	50.789	1.00	67.70	AAAA
ATOM	2688	OE1	GLU	A	337	20.319	52.554	50.851	1.00	67.05	AAAA
ATOM	2689	OE2	GLU	A	337	19.711	50.518	51.398	1.00	67.79	AAAA
ATOM	2690	C	GLU	A	337	18.322	50.222	46.827	1.00	69.28	AAAA
ATOM	2691	O	GLU	A	337	17.886	50.705	45.780	1.00	69.50	AAAA
ATOM	2692	N	PHE	A	338	17.966	49.012	47.259	1.00	69.55	AAAA
ATOM	2693	CA	PHE	A	338	17.035	48.176	46.497	1.00	69.67	AAAA
ATOM	2694	CB	PHE	A	338	16.995	46.759	47.066	1.00	70.51	AAAA
ATOM	2695	CG	PHE	A	338	16.225	45.789	46.221	1.00	71.57	AAAA
ATOM	2696	CD1	PHE	A	338	16.666	45.462	44.936	1.00	72.04	AAAA
ATOM	2697	CD2	PHE	A	338	15.052	45.208	46.698	1.00	71.69	AAAA
ATOM	2698	CE1	PHE	A	338	15.944	44.566	44.138	1.00	72.23	AAAA
ATOM	2699	CE2	PHE	A	338	14.323	44.313	45.909	1.00	71.93	AAAA
ATOM	2700	CZ	PHE	A	338	14.770	43.991	44.627	1.00	72.11	AAAA
ATOM	2701	C	PHE	A	338	15.633	48.770	46.494	1.00	69.26	AAAA
ATOM	2702	O	PHE	A	338	15.072	49.029	45.434	1.00	68.86	AAAA
ATOM	2703	N	ASP	A	339	15.053	48.962	47.674	1.00	69.35	AAAA
ATOM	2704	CA	ASP	A	339	13.733	49.572	47.755	1.00	69.61	AAAA
ATOM	2705	CB	ASP	A	339	13.134	49.457	49.157	1.00	69.48	AAAA
ATOM	2706	CG	ASP	A	339	11.819	50.233	49.299	1.00	69.72	AAAA

257/263

Figure 19-42

ATOM	2707	OD1	ASP	A	339	11.813	51.462	49.058	1.00	69.39	AAAA
ATOM	2708	OD2	ASP	A	339	10.790	49.618	49.655	1.00	69.78	AAAA
ATOM	2709	C	ASP	A	339	13.972	51.035	47.440	1.00	69.95	AAAA
ATOM	2710	O	ASP	A	339	14.305	51.815	48.333	1.00	69.92	AAAA
ATOM	2711	N	ASP	A	340	13.810	51.389	46.168	1.00	70.23	AAAA
ATOM	2712	CA	ASP	A	340	14.023	52.748	45.699	1.00	70.39	AAAA
ATOM	2713	CB	ASP	A	340	12.757	53.283	45.041	1.00	70.64	AAAA
ATOM	2714	CG	ASP	A	340	12.397	52.517	43.791	1.00	70.86	AAAA
ATOM	2715	OD1	ASP	A	340	12.126	51.302	43.903	1.00	70.93	AAAA
ATOM	2716	OD2	ASP	A	340	12.399	53.125	42.699	1.00	70.89	AAAA
ATOM	2717	C	ASP	A	340	14.482	53.674	46.807	1.00	70.63	AAAA
ATOM	2718	O	ASP	A	340	15.688	53.847	47.008	1.00	71.13	AAAA
ATOM	2719	N	GLU	A	341	13.543	54.259	47.544	1.00	69.95	AAAA
ATOM	2720	CA	GLU	A	341	13.947	55.150	48.619	1.00	69.17	AAAA
ATOM	2721	CB	GLU	A	341	13.636	56.613	48.266	1.00	70.83	AAAA
ATOM	2722	CG	GLU	A	341	14.098	57.601	49.347	1.00	73.44	AAAA
ATOM	2723	CD	GLU	A	341	13.956	59.071	48.951	1.00	75.27	AAAA
ATOM	2724	OE1	GLU	A	341	12.825	59.518	48.646	1.00	76.21	AAAA
ATOM	2725	OE2	GLU	A	341	14.984	59.786	48.954	1.00	75.69	AAAA
ATOM	2726	C	GLU	A	341	13.367	54.819	49.983	1.00	67.09	AAAA
ATOM	2727	O	GLU	A	341	12.233	55.176	50.297	1.00	66.57	AAAA
ATOM	2728	N	VAL	A	342	14.158	54.114	50.785	1.00	64.87	AAAA
ATOM	2729	CA	VAL	A	342	13.767	53.779	52.148	1.00	62.55	AAAA
ATOM	2730	CB	VAL	A	342	14.265	52.377	52.589	1.00	62.81	AAAA
ATOM	2731	CG1	VAL	A	342	14.042	52.193	54.081	1.00	62.56	AAAA
ATOM	2732	CG2	VAL	A	342	13.513	51.298	51.849	1.00	63.69	AAAA
ATOM	2733	C	VAL	A	342	14.483	54.822	52.982	1.00	59.94	AAAA
ATOM	2734	O	VAL	A	342	14.022	55.215	54.054	1.00	59.91	AAAA
ATOM	2735	N	ASP	A	343	15.609	55.278	52.442	1.00	56.85	AAAA
ATOM	2736	CA	ASP	A	343	16.457	56.266	53.085	1.00	54.01	AAAA
ATOM	2737	CB	ASP	A	343	15.639	57.446	53.605	1.00	54.18	AAAA
ATOM	2738	CG	ASP	A	343	16.505	58.511	54.241	1.00	53.96	AAAA
ATOM	2739	OD1	ASP	A	343	15.947	59.485	54.785	1.00	54.59	AAAA
ATOM	2740	OD2	ASP	A	343	17.747	58.373	54.191	1.00	53.61	AAAA
ATOM	2741	C	ASP	A	343	17.186	55.609	54.242	1.00	51.92	AAAA
ATOM	2742	O	ASP	A	343	16.611	55.371	55.307	1.00	51.89	AAAA
ATOM	2743	N	ARG	A	344	18.458	55.306	54.029	1.00	48.86	AAAA
ATOM	2744	CA	ARG	A	344	19.240	54.676	55.069	1.00	45.59	AAAA
ATOM	2745	CB	ARG	A	344	19.847	53.369	54.573	1.00	43.94	AAAA
ATOM	2746	CG	ARG	A	344	18.847	52.289	54.220	1.00	41.70	AAAA
ATOM	2747	CD	ARG	A	344	17.953	51.955	55.385	1.00	38.94	AAAA
ATOM	2748	NE	ARG	A	344	17.139	50.781	55.096	1.00	36.78	AAAA
ATOM	2749	CZ	ARG	A	344	16.176	50.316	55.888	1.00	34.81	AAAA
ATOM	2750	NH1	ARG	A	344	15.890	50.927	57.033	1.00	34.11	AAAA
ATOM	2751	NH2	ARG	A	344	15.506	49.228	55.537	1.00	31.84	AAAA
ATOM	2752	C	ARG	A	344	20.340	55.604	55.520	1.00	44.83	AAAA
ATOM	2753	O	ARG	A	344	21.308	55.157	56.128	1.00	43.97	AAAA
ATOM	2754	N	SER	A	345	20.192	56.895	55.226	1.00	44.32	AAAA
ATOM	2755	CA	SER	A	345	21.199	57.877	55.618	1.00	43.74	AAAA
ATOM	2756	CB	SER	A	345	20.860	59.248	55.039	1.00	44.49	AAAA
ATOM	2757	OG	SER	A	345	19.645	59.729	55.577	1.00	46.07	AAAA
ATOM	2758	C	SER	A	345	21.307	57.977	57.144	1.00	42.82	AAAA
ATOM	2759	O	SER	A	345	22.304	58.472	57.674	1.00	42.91	AAAA
ATOM	2760	N	TYR	A	346	20.282	57.509	57.849	1.00	41.48	AAAA
ATOM	2761	CA	TYR	A	346	20.296	57.549	59.303	1.00	40.35	AAAA
ATOM	2762	CB	TYR	A	346	18.947	57.068	59.858	1.00	40.38	AAAA
ATOM	2763	CG	TYR	A	346	18.630	55.601	59.609	1.00	39.28	AAAA
ATOM	2764	CD1	TYR	A	346	19.293	54.589	60.316	1.00	38.74	AAAA
ATOM	2765	CE1	TYR	A	346	19.022	53.243	60.079	1.00	37.71	AAAA
ATOM	2766	CD2	TYR	A	346	17.682	55.225	58.653	1.00	38.49	AAAA
ATOM	2767	CE2	TYR	A	346	17.405	53.882	58.408	1.00	38.17	AAAA
ATOM	2768	CZ	TYR	A	346	18.079	52.899	59.126	1.00	37.59	AAAA
ATOM	2769	OH	TYR	A	346	17.794	51.580	58.898	1.00	37.14	AAAA
ATOM	2770	C	TYR	A	346	21.436	56.686	59.849	1.00	39.91	AAAA
ATOM	2771	O	TYR	A	346	21.967	56.957	60.921	1.00	40.28	AAAA
ATOM	2772	N	MET	A	347	21.800	55.640	59.113	1.00	39.14	AAAA

258/263

Figure 19-43

ATOM	2773	CA	MET	A	347	22.879	54.756	59.530	1.00	38.19	AAAA
ATOM	2774	CB	MET	A	347	23.042	53.582	58.566	1.00	38.26	AAAA
ATOM	2775	CG	MET	A	347	21.973	52.523	58.694	1.00	38.17	AAAA
ATOM	2776	SD	MET	A	347	22.317	51.115	57.641	1.00	38.05	AAAA
ATOM	2777	CE	MET	A	347	22.237	51.892	56.101	1.00	37.61	AAAA
ATOM	2778	C	MET	A	347	24.189	55.494	59.603	1.00	38.00	AAAA
ATOM	2779	O	MET	A	347	25.127	55.033	60.250	1.00	37.40	AAAA
ATOM	2780	N	LEU	A	348	24.248	56.637	58.929	1.00	38.08	AAAA
ATOM	2781	CA	LEU	A	348	25.449	57.463	58.898	1.00	38.07	AAAA
ATOM	2782	CB	LEU	A	348	25.445	58.330	57.638	1.00	36.66	AAAA
ATOM	2783	CG	LEU	A	348	25.379	57.583	56.310	1.00	35.47	AAAA
ATOM	2784	CD1	LEU	A	348	25.285	58.559	55.165	1.00	34.51	AAAA
ATOM	2785	CD2	LEU	A	348	26.605	56.716	56.167	1.00	36.56	AAAA
ATOM	2786	C	LEU	A	348	25.521	58.353	60.138	1.00	39.07	AAAA
ATOM	2787	O	LEU	A	348	26.546	58.980	60.406	1.00	38.81	AAAA
ATOM	2788	N	GLU	A	349	24.432	58.385	60.898	1.00	39.90	AAAA
ATOM	2789	CA	GLU	A	349	24.363	59.213	62.092	1.00	40.95	AAAA
ATOM	2790	CB	GLU	A	349	22.961	59.821	62.203	1.00	41.70	AAAA
ATOM	2791	CG	GLU	A	349	22.515	60.629	60.966	1.00	42.28	AAAA
ATOM	2792	CD	GLU	A	349	23.349	61.891	60.708	1.00	42.51	AAAA
ATOM	2793	OE1	GLU	A	349	23.414	62.778	61.587	1.00	42.38	AAAA
ATOM	2794	OE2	GLU	A	349	23.933	61.998	59.614	1.00	43.34	AAAA
ATOM	2795	C	GLU	A	349	24.740	58.511	63.406	1.00	41.12	AAAA
ATOM	2796	O	GLU	A	349	24.664	59.118	64.476	1.00	41.38	AAAA
ATOM	2797	N	THR	A	350	25.140	57.243	63.326	1.00	40.86	AAAA
ATOM	2798	CA	THR	A	350	25.555	56.475	64.504	1.00	40.69	AAAA
ATOM	2799	CB	THR	A	350	24.405	56.283	65.510	1.00	41.56	AAAA
ATOM	2800	CG1	THR	A	350	24.062	57.549	66.078	1.00	41.48	AAAA
ATOM	2801	CG2	THR	A	350	24.821	55.345	66.638	1.00	41.19	AAAA
ATOM	2802	C	THR	A	350	26.109	55.109	64.141	1.00	40.14	AAAA
ATOM	2803	O	THR	A	350	25.857	54.595	63.055	1.00	39.93	AAAA
ATOM	2804	N	LEU	A	351	26.865	54.527	65.067	1.00	40.32	AAAA
ATOM	2805	CA	LEU	A	351	27.491	53.227	64.857	1.00	40.70	AAAA
ATOM	2806	CB	LEU	A	351	28.855	53.213	65.540	1.00	39.89	AAAA
ATOM	2807	CG	LEU	A	351	29.911	52.290	64.951	1.00	39.68	AAAA
ATOM	2808	CD1	LEU	A	351	31.170	52.403	65.772	1.00	39.88	AAAA
ATOM	2809	CD2	LEU	A	351	29.414	50.861	64.945	1.00	40.70	AAAA
ATOM	2810	C	LEU	A	351	26.612	52.091	65.384	1.00	41.12	AAAA
ATOM	2811	O	LEU	A	351	26.467	51.060	64.736	1.00	40.02	AAAA
ATOM	2812	N	LYS	A	352	26.040	52.292	66.567	1.00	42.99	AAAA
ATOM	2813	CA	LYS	A	352	25.138	51.326	67.201	1.00	43.93	AAAA
ATOM	2814	CB	LYS	A	352	25.412	51.225	68.707	1.00	43.38	AAAA
ATOM	2815	CG	LYS	A	352	26.743	50.597	69.055	1.00	44.68	AAAA
ATOM	2816	CD	LYS	A	352	27.185	50.927	70.482	1.00	45.48	AAAA
ATOM	2817	CE	LYS	A	352	26.189	50.500	71.539	1.00	46.21	AAAA
ATOM	2818	NZ	LYS	A	352	26.646	50.944	72.895	1.00	47.34	AAAA
ATOM	2819	C	LYS	A	352	23.723	51.838	67.003	1.00	44.40	AAAA
ATOM	2820	O	LYS	A	352	23.375	52.917	67.488	1.00	45.79	AAAA
ATOM	2821	N	ASP	A	353	22.904	51.083	66.287	1.00	44.78	AAAA
ATOM	2822	CA	ASP	A	353	21.532	51.509	66.074	1.00	44.79	AAAA
ATOM	2823	CB	ASP	A	353	21.050	51.030	64.702	1.00	45.20	AAAA
ATOM	2824	CG	ASP	A	353	21.146	49.544	64.546	1.00	45.21	AAAA
ATOM	2825	OD1	ASP	A	353	21.806	49.086	63.581	1.00	45.06	AAAA
ATOM	2826	OD2	ASP	A	353	20.549	48.841	65.391	1.00	45.54	AAAA
ATOM	2827	C	ASP	A	353	20.645	50.993	67.217	1.00	44.44	AAAA
ATOM	2828	O	ASP	A	353	21.042	50.113	67.973	1.00	44.29	AAAA
ATOM	2829	N	PRO	A	354	19.439	51.553	67.367	1.00	44.22	AAAA
ATOM	2830	CD	PRO	A	354	18.839	52.617	66.550	1.00	44.38	AAAA
ATOM	2831	CA	PRO	A	354	18.500	51.163	68.419	1.00	44.18	AAAA
ATOM	2832	CB	PRO	A	354	17.371	52.170	68.238	1.00	44.52	AAAA
ATOM	2833	CG	PRO	A	354	17.368	52.341	66.749	1.00	44.66	AAAA
ATOM	2834	C	PRO	A	354	17.995	49.740	68.328	1.00	43.87	AAAA
ATOM	2835	O	PRO	A	354	17.962	49.152	67.249	1.00	44.48	AAAA
ATOM	2836	N	TRP	A	355	17.588	49.198	69.469	1.00	43.23	AAAA
ATOM	2837	CA	TRP	A	355	17.051	47.851	69.500	1.00	42.88	AAAA
ATOM	2838	CB	TRP	A	355	16.743	47.401	70.927	1.00	46.42	AAAA

259/263
Figure 19-44

ATOM	2839	CG	TRP	A	355	17.959	47.052	71.695	1.00	49.91	AAAA
ATOM	2840	CD2	TBP	A	355	18.476	45.733	71.903	1.00	51.56	AAAA
ATOM	2841	CE2	TRP	A	355	19.684	45.868	72.627	1.00	52.03	AAAA
ATOM	2842	CE3	TRP	A	355	18.038	44.450	71.548	1.00	52.25	AAAA
ATOM	2843	CD1	TRP	A	355	18.846	47.915	72.284	1.00	50.53	AAAA
ATOM	2844	NE1	TRP	A	355	19.885	47.208	72.846	1.00	51.63	AAAA
ATOM	2845	CZ2	TRP	A	355	20.460	44.763	73.003	1.00	52.64	AAAA
ATOM	2846	CZ3	TRP	A	355	18.810	43.352	71.921	1.00	53.12	AAAA
ATOM	2847	CH2	TRP	A	355	20.008	43.518	72.642	1.00	53.02	AAAA
ATOM	2848	C	TRP	A	355	15.788	47.767	68.675	1.00	40.28	AAAA
ATOM	2849	O	TRP	A	355	15.017	48.720	68.591	1.00	39.82	AAAA
ATOM	2850	N	ARG	A	356	15.591	46.610	68.065	1.00	36.83	AAAA
ATOM	2851	CA	ARG	A	356	14.440	46.365	67.225	1.00	33.70	AAAA
ATOM	2852	CB	ARG	A	356	14.901	46.197	65.772	1.00	29.50	AAAA
ATOM	2853	CG	ARG	A	356	15.635	47.423	65.256	1.00	25.22	AAAA
ATOM	2854	CD	ARG	A	356	16.418	47.194	63.973	1.00	21.53	AAAA
ATOM	2855	NE	ARG	A	356	17.055	48.435	63.533	1.00	18.55	AAAA
ATOM	2856	CZ	ARG	A	356	17.976	48.533	62.574	1.00	17.06	AAAA
ATOM	2857	NH1	ARG	A	356	18.403	47.451	61.919	1.00	17.64	AAAA
ATOM	2858	NH2	ARG	A	356	18.445	49.721	62.241	1.00	11.56	AAAA
ATOM	2859	C	ARG	A	356	13.831	45.095	67.773	1.00	34.63	AAAA
ATOM	2860	O	ARG	A	356	13.605	44.117	67.051	1.00	35.86	AAAA
ATOM	2861	N	GLY	A	357	13.587	45.112	69.079	1.00	34.58	AAAA
ATOM	2862	CA	GLY	A	357	13.003	43.960	69.734	1.00	34.33	AAAA
ATOM	2863	C	GLY	A	357	11.536	43.783	69.395	1.00	34.31	AAAA
ATOM	2864	O	GLY	A	357	11.006	44.418	68.484	1.00	33.56	AAAA
ATOM	2865	N	GLY	A	358	10.876	42.906	70.139	1.00	34.47	AAAA
ATOM	2866	CA	GLY	A	358	9.468	42.656	69.916	1.00	34.61	AAAA
ATOM	2867	C	GLY	A	358	9.114	41.389	70.655	1.00	34.47	AAAA
ATOM	2868	O	GLY	A	358	9.962	40.821	71.345	1.00	34.27	AAAA
ATOM	2869	N	GLU	A	359	7.869	40.948	70.523	1.00	34.16	AAAA
ATOM	2870	CA	GLU	A	359	7.438	39.729	71.180	1.00	33.94	AAAA
ATOM	2871	CB	GLU	A	359	5.910	39.644	71.174	1.00	34.78	AAAA
ATOM	2872	CG	GLU	A	359	5.278	40.648	72.123	1.00	36.70	AAAA
ATOM	2873	CD	GLU	A	359	3.863	41.020	71.740	1.00	38.40	AAAA
ATOM	2874	OE1	GLU	A	359	3.017	40.108	71.600	1.00	39.65	AAAA
ATOM	2875	OE2	GLU	A	359	3.598	42.234	71.584	1.00	38.52	AAAA
ATOM	2876	C	GLU	A	359	8.058	38.549	70.464	1.00	32.86	AAAA
ATOM	2877	O	GLU	A	359	8.678	38.692	69.427	1.00	32.92	AAAA
ATOM	2878	N	VAL	A	360	7.918	37.375	71.036	1.00	32.63	AAAA
ATOM	2879	CA	VAL	A	360	8.480	36.215	70.409	1.00	32.70	AAAA
ATOM	2880	CB	VAL	A	360	9.422	35.472	71.376	1.00	33.24	AAAA
ATOM	2881	CG1	VAL	A	360	10.017	34.252	70.701	1.00	32.99	AAAA
ATOM	2882	CG2	VAL	A	360	10.521	36.406	71.827	1.00	32.09	AAAA
ATOM	2883	C	VAL	A	360	7.339	35.319	69.976	1.00	32.81	AAAA
ATOM	2884	O	VAL	A	360	6.702	34.660	70.791	1.00	32.02	AAAA
ATOM	2885	N	ARG	A	361	7.084	35.321	68.674	1.00	33.12	AAAA
ATOM	2886	CA	ARG	A	361	6.035	34.508	68.086	1.00	33.52	AAAA
ATOM	2887	CB	ARG	A	361	6.148	34.558	66.565	1.00	33.43	AAAA
ATOM	2888	CG	ARG	A	361	5.731	35.885	65.967	1.00	34.35	AAAA
ATOM	2889	CD	ARG	A	361	6.041	35.972	64.469	1.00	33.90	AAAA
ATOM	2890	NE	ARG	A	361	7.430	36.331	64.193	1.00	31.70	AAAA
ATOM	2891	CZ	ARG	A	361	7.890	36.608	62.978	1.00	31.18	AAAA
ATOM	2892	NH1	ARG	A	361	7.068	36.562	61.941	1.00	30.48	AAAA
ATOM	2893	NH2	ARG	A	361	9.162	36.948	62.802	1.00	29.71	AAAA
ATOM	2894	C	ARG	A	361	6.066	33.057	68.557	1.00	34.20	AAAA
ATOM	2895	O	ARG	A	361	7.101	32.537	68.968	1.00	33.79	AAAA
ATOM	2896	N	LYS	A	362	4.914	32.407	68.496	1.00	34.68	AAAA
ATOM	2897	CA	LYS	A	362	4.808	31.022	68.901	1.00	35.62	AAAA
ATOM	2898	CB	LYS	A	362	3.350	30.555	68.782	1.00	37.80	AAAA
ATOM	2899	CG	LYS	A	362	2.378	31.226	69.756	1.00	40.38	AAAA
ATOM	2900	CD	LYS	A	362	2.505	32.777	69.777	1.00	42.09	AAAA
ATOM	2901	CE	LYS	A	362	2.208	33.446	68.420	1.00	41.94	AAAA
ATOM	2902	NZ	LYS	A	362	2.473	34.909	68.451	1.00	39.85	AAAA
ATOM	2903	C	LYS	A	362	5.710	30.177	68.005	1.00	35.12	AAAA
ATOM	2904	O	LYS	A	362	6.425	29.301	68.487	1.00	34.14	AAAA

ATOM	2905	N	GLU	A	363	5.661	30.460	66.703	1.00	35.12	AAAA
ATOM	2906	CA	GLU	A	363	6.445	29.741	65.699	1.00	35.62	AAAA
ATOM	2907	CB	GLU	A	363	6.567	30.560	64.424	1.00	36.81	AAAA
ATOM	2908	CG	GLU	A	363	5.280	30.808	63.711	1.00	38.66	AAAA
ATOM	2909	CD	GLU	A	363	5.477	31.704	62.517	1.00	39.60	AAAA
ATOM	2910	OE1	GLU	A	363	6.287	31.324	61.637	1.00	39.11	AAAA
ATOM	2911	OE2	GLU	A	363	4.826	32.782	62.469	1.00	39.95	AAAA
ATOM	2912	C	GLU	A	363	7.836	29.450	66.181	1.00	35.14	AAAA
ATOM	2913	O	GLU	A	363	8.321	28.316	66.098	1.00	34.50	AAAA
ATOM	2914	N	VAL	A	364	8.475	30.505	66.671	1.00	34.96	AAAA
ATOM	2915	CA	VAL	A	364	9.830	30.431	67.180	1.00	34.44	AAAA
ATOM	2916	CB	VAL	A	364	10.338	31.821	67.570	1.00	33.68	AAAA
ATOM	2917	CG1	VAL	A	364	11.739	31.722	68.162	1.00	34.13	AAAA
ATOM	2918	CG2	VAL	A	364	10.337	32.715	66.347	1.00	31.83	AAAA
ATOM	2919	C	VAL	A	364	9.908	29.499	68.370	1.00	34.44	AAAA
ATOM	2920	O	VAL	A	364	10.789	28.640	68.430	1.00	36.01	AAAA
ATOM	2921	N	LYS	A	365	8.980	29.649	69.305	1.00	33.27	AAAA
ATOM	2922	CA	LYS	A	365	8.970	28.790	70.476	1.00	33.20	AAAA
ATOM	2923	CB	LYS	A	365	7.968	29.319	71.508	1.00	34.28	AAAA
ATOM	2924	CG	LYS	A	365	8.307	30.705	72.033	1.00	33.67	AAAA
ATOM	2925	CD	LYS	A	365	7.282	31.181	73.039	1.00	34.85	AAAA
ATOM	2926	CE	LYS	A	365	7.658	32.534	73.638	1.00	36.47	AAAA
ATOM	2927	NZ	LYS	A	365	6.698	32.990	74.710	1.00	37.91	AAAA
ATOM	2928	C	LYS	A	365	8.654	27.342	70.109	1.00	32.75	AAAA
ATOM	2929	O	LYS	A	365	9.071	26.421	70.818	1.00	31.95	AAAA
ATOM	2930	N	ASP	A	366	7.919	27.136	69.012	1.00	32.81	AAAA
ATOM	2931	CA	ASP	A	366	7.600	25.777	68.581	1.00	33.65	AAAA
ATOM	2932	CB	ASP	A	366	6.459	25.726	67.557	1.00	33.98	AAAA
ATOM	2933	CG	ASP	A	366	5.131	26.107	68.140	1.00	33.94	AAAA
ATOM	2934	OD1	ASP	A	366	4.870	25.767	69.307	1.00	33.89	AAAA
ATOM	2935	OD2	ASP	A	366	4.332	26.722	67.412	1.00	35.08	AAAA
ATOM	2936	C	ASP	A	366	8.820	25.167	67.940	1.00	33.05	AAAA
ATOM	2937	O	ASP	A	366	9.140	24.006	68.172	1.00	33.66	AAAA
ATOM	2938	N	THR	A	367	9.473	25.959	67.102	1.00	33.07	AAAA
ATOM	2939	CA	THR	A	367	10.684	25.540	66.412	1.00	32.27	AAAA
ATOM	2940	CB	THR	A	367	11.304	26.719	65.641	1.00	32.28	AAAA
ATOM	2941	OG1	THR	A	367	10.473	27.039	64.520	1.00	30.64	AAAA
ATOM	2942	CG2	THR	A	367	12.711	26.377	65.166	1.00	33.29	AAAA
ATOM	2943	C	THR	A	367	11.680	25.044	67.442	1.00	31.71	AAAA
ATOM	2944	O	THR	A	367	12.178	23.918	67.352	1.00	30.45	AAAA
ATOM	2945	N	LEU	A	368	11.955	25.896	68.426	1.00	32.05	AAAA
ATOM	2946	CA	LEU	A	368	12.888	25.560	69.482	1.00	32.49	AAAA
ATOM	2947	CB	LEU	A	368	13.085	26.749	70.421	1.00	32.27	AAAA
ATOM	2948	CG	LEU	A	368	14.097	27.809	69.960	1.00	32.71	AAAA
ATOM	2949	CD1	LEU	A	368	15.488	27.170	69.899	1.00	33.00	AAAA
ATOM	2950	CD2	LEU	A	368	13.709	28.393	68.597	1.00	31.86	AAAA
ATOM	2951	C	LEU	A	368	12.455	24.334	70.256	1.00	33.82	AAAA
ATOM	2952	O	LEU	A	368	13.266	23.133	70.489	1.00	34.29	AAAA
ATOM	2953	N	GLU	A	369	11.183	24.285	70.645	1.00	34.30	AAAA
ATOM	2954	CA	GLU	A	369	10.687	23.135	71.375	1.00	36.07	AAAA
ATOM	2955	CB	GLU	A	369	9.211	23.319	71.748	1.00	38.71	AAAA
ATOM	2956	CG	GLU	A	369	8.974	24.285	72.920	1.00	40.18	AAAA
ATOM	2957	CD	GLU	A	369	7.509	24.359	73.341	1.00	41.56	AAAA
ATOM	2958	OE1	GLU	A	369	6.917	23.276	73.572	1.00	41.83	AAAA
ATOM	2959	OE2	GLU	A	369	6.957	25.489	73.451	1.00	41.74	AAAA
ATOM	2960	C	GLU	A	369	10.893	21.822	70.611	1.00	37.16	AAAA
ATOM	2961	O	GLU	A	369	11.338	20.831	71.196	1.00	37.00	AAAA
ATOM	2962	N	LYS	A	370	10.586	21.788	69.315	1.00	37.71	AAAA
ATOM	2963	CA	LYS	A	370	10.797	20.547	68.567	1.00	38.46	AAAA
ATOM	2964	CB	LYS	A	370	10.166	20.604	67.177	1.00	39.96	AAAA
ATOM	2965	CG	LYS	A	370	8.646	20.532	67.186	1.00	42.68	AAAA
ATOM	2966	CD	LYS	A	370	8.092	20.320	65.775	1.00	44.54	AAAA
ATOM	2967	CE	LYS	A	370	6.572	20.075	65.781	1.00	45.55	AAAA
ATOM	2968	NZ	LYS	A	370	6.009	19.797	64.409	1.00	45.50	AAAA
ATOM	2969	C	LYS	A	370	12.282	20.235	68.452	1.00	38.34	AAAA
ATOM	2970	O	LYS	A	370	12.683	19.071	68.493	1.00	37.86	AAAA

261/263 Figure 19-46

ATOM	2971	N	ALA	A	371	13.105	21.266	68.311	1.00	37.69	AAAA
ATOM	2972	CA	ALA	A	371	14.543	21.057	68.226	1.00	37.20	AAAA
ATOM	2973	CB	ALA	A	371	15.258	22.375	67.936	1.00	35.48	AAAA
ATOM	2974	C	ALA	A	371	15.023	20.477	69.558	1.00	37.63	AAAA
ATOM	2975	O	ALA	A	371	15.920	19.626	69.585	1.00	37.12	AAAA
ATOM	2976	N	LYS	A	372	14.426	20.930	70.665	1.00	37.59	AAAA
ATOM	2977	CA	LYS	A	372	14.796	20.432	71.995	1.00	37.46	AAAA
ATOM	2978	CB	LYS	A	372	14.022	21.156	73.095	1.00	36.52	AAAA
ATOM	2979	CG	LYS	A	372	14.287	22.634	73.111	1.00	22.67	AAAA
ATOM	2980	CD	LYS	A	372	13.309	23.396	74.022	1.00	22.67	AAAA
ATOM	2981	CE	LYS	A	372	13.600	24.874	73.901	1.00	22.67	AAAA
ATOM	2982	NZ	LYS	A	372	12.692	25.708	74.785	1.00	22.67	AAAA
ATOM	2983	C	LYS	A	372	14.495	18.957	72.077	1.00	37.60	AAAA
ATOM	2984	O	LYS	A	372	15.367	18.171	72.407	1.00	37.26	AAAA
ATOM	2985	N	ALA	A	373	13.249	18.595	71.789	1.00	38.17	AAAA
ATOM	2986	CA	ALA	A	373	12.812	17.206	71.829	1.00	39.55	AAAA
ATOM	2987	CB	ALA	A	373	11.365	17.109	71.395	1.00	39.34	AAAA
ATOM	2988	C	ALA	A	373	13.675	16.277	70.972	1.00	41.02	AAAA
ATOM	2989	O	ALA	A	373	14.366	15.410	71.561	1.00	42.26	AAAA
ATOM	2990	OXT	ALA	A	373	13.663	16.416	69.725	1.00	42.06	AAAA
HETATM	2991	ZN	ZN	B	951	23.696	34.788	54.072	1.00	27.38	ZONE
HETATM	2992	O1	SHA	C	1	24.578	33.295	53.458	1.00	31.95	SAHA
HETATM	2993	O2	SHA	C	1	24.294	35.218	51.444	1.00	33.51	SAHA
HETATM	2994	N1	SHA	C	1	24.578	33.085	52.069	1.00	34.03	SAHA
HETATM	2995	C1	SHA	C	1	24.063	34.053	51.246	1.00	34.25	SAHA
HETATM	2996	C2	SHA	C	1	23.090	33.625	50.259	1.00	36.87	SAHA
HETATM	2997	C3	SHA	C	1	23.548	33.781	48.816	1.00	39.33	SAHA
HETATM	2998	C4	SHA	C	1	22.498	33.274	47.852	1.00	40.86	SAHA
HETATM	2999	C5	SHA	C	1	21.590	34.413	47.455	1.00	43.37	SAHA
HETATM	3000	C6	SHA	C	1	21.061	34.017	46.092	1.00	46.72	SAHA
HETATM	3001	C7	SHA	C	1	19.754	34.714	45.787	1.00	48.75	SAHA
HETATM	3002	C8	SHA	C	1	19.960	35.720	44.693	1.00	50.75	SAHA
HETATM	3003	O3	SHA	C	1	20.381	35.467	43.575	1.00	51.08	SAHA
HETATM	3004	N2	SHA	C	1	19.591	36.956	45.085	1.00	52.52	SAHA
HETATM	3005	C9	SHA	C	1	19.842	38.330	44.507	1.00	54.25	SAHA
HETATM	3006	C10	SHA	C	1	19.243	39.431	45.215	1.00	55.76	SAHA
HETATM	3007	C11	SHA	C	1	19.423	40.804	44.727	1.00	56.53	SAHA
HETATM	3008	C12	SHA	C	1	20.169	41.085	43.545	1.00	56.58	SAHA
HETATM	3009	C13	SHA	C	1	20.755	39.942	42.827	1.00	55.93	SAHA
HETATM	3010	C14	SHA	C	1	20.612	38.546	43.304	1.00	54.65	SAHA
HETATM	3011	OH2	WAT	D	2	36.485	44.023	49.378	1.00	4.67	SOLV
HETATM	3012	OH2	WAT	D	3	27.702	16.865	62.162	1.00	4.67	SOLV
HETATM	3013	OH2	WAT	D	4	23.251	30.387	59.575	1.00	10.12	SOLV
HETATM	3014	OH2	WAT	D	5	33.825	41.862	46.926	1.00	21.13	SOLV
HETATM	3015	OH2	WAT	D	6	24.866	44.453	47.867	1.00	23.72	SOLV
HETATM	3016	OH2	WAT	D	7	34.145	20.442	33.590	1.00	18.19	SOLV
HETATM	3017	OH2	WAT	D	8	7.921	29.753	62.099	1.00	20.79	SOLV
HETATM	3018	OH2	WAT	D	9	17.863	6.978	64.018	1.00	28.94	SOLV
HETATM	3019	OH2	WAT	D	10	35.580	44.610	74.823	1.00	31.62	SOLV
HETATM	3020	OH2	WAT	D	11	49.208	27.797	65.303	1.00	14.70	SOLV
HETATM	3021	OH2	WAT	D	12	20.490	34.049	61.067	1.00	25.01	SOLV
HETATM	3022	OH2	WAT	D	13	44.757	33.106	46.084	1.00	25.90	SOLV
HETATM	3023	OH2	WAT	D	14	22.457	60.823	57.444	1.00	15.21	SOLV
HETATM	3024	OH2	WAT	D	15	3.399	32.742	65.163	1.00	20.66	SOLV
HETATM	3025	OH2	WAT	D	16	32.273	51.414	45.610	1.00	22.37	SOLV
HETATM	3026	OH2	WAT	D	17	26.328	42.873	73.427	1.00	27.86	SOLV
HETATM	3027	OH2	WAT	D	18	48.249	24.121	56.778	1.00	15.09	SOLV
HETATM	3028	OH2	WAT	D	19	15.249	44.552	72.082	1.00	40.95	SOLV
HETATM	3029	OH2	WAT	D	20	26.444	9.269	52.633	1.00	26.66	SOLV
HETATM	3030	OH2	WAT	D	21	26.554	18.383	59.650	1.00	11.42	SOLV
HETATM	3031	OH2	WAT	D	22	39.456	25.964	72.316	1.00	20.32	SOLV
HETATM	3032	OH2	WAT	D	23	26.743	37.600	38.359	1.00	37.22	SOLV
HETATM	3033	OH2	WAT	D	24	44.666	23.818	39.068	1.00	32.27	SOLV
HETATM	3034	OH2	WAT	D	25	14.714	52.213	70.663	1.00	29.24	SOLV
HETATM	3035	OH2	WAT	D	26	45.129	18.856	69.864	1.00	29.58	SOLV
HETATM	3036	OH2	WAT	D	27	30.024	17.886	49.758	1.00	15.52	SOLV

HETATM 3037	OH2 WAT D	28.	20.659	28.788	43.520	1.00	28.55	SOLV
HETATM 3038	OH2 WAT D	29	32.271	38.000	53.512	1.00	47.72	SOLV
HETATM 3039	OH2 WAT D	30	18.285	29.333	54.536	1.00	21.34	SOLV
HETATM 3040	OH2 WAT D	31	49.978	38.669	73.461	1.00	31.02	SOLV
HETATM 3041	OH2 WAT D	32	21.587	50.386	71.043	1.00	14.52	SOLV
HETATM 3042	OH2 WAT D	33	46.784	32.121	33.375	1.00	31.79	SOLV
HETATM 3043	OH2 WAT D	34	33.359	39.755	49.117	1.00	16.13	SOLV
HETATM 3044	OH2 WAT D	35	7.687	37.657	51.568	1.00	27.22	SOLV
HETATM 3045	OH2 WAT D	36	44.238	35.392	33.961	1.00	19.67	SOLV
HETATM 3046	OH2 WAT D	37	10.908	25.384	58.206	1.00	33.51	SOLV
HETATM 3047	OH2 WAT D	38	36.758	27.243	70.552	1.00	39.61	SOLV
HETATM 3048	OH2 WAT D	39	45.825	46.691	54.654	1.00	32.43	SOLV
HETATM 3049	OH2 WAT D	40	52.489	20.282	52.165	1.00	39.37	SOLV
HETATM 3050	OH2 WAT D	42	12.117	17.831	56.596	1.00	27.74	SOLV
HETATM 3051	OH2 WAT D	43	45.023	26.168	35.172	1.00	14.09	SOLV
HETATM 3052	OH2 WAT D	44	39.392	12.771	62.066	1.00	35.15	SOLV
HETATM 3053	OH2 WAT D	45	3.930	26.970	63.814	1.00	22.23	SOLV
HETATM 3054	OH2 WAT D	46	8.454	19.321	71.677	1.00	32.36	SOLV
HETATM 3055	OH2 WAT D	47	20.280	18.126	73.237	1.00	33.88	SOLV
HETATM 3056	OH2 WAT D	48	9.321	39.409	54.873	1.00	18.57	SOLV
HETATM 3057	OH2 WAT D	49	50.852	41.323	58.048	1.00	21.25	SOLV
HETATM 3058	OH2 WAT D	50	37.134	34.599	60.315	1.00	61.70	SOLV
HETATM 3059	OH2 WAT D	51	14.944	62.815	48.613	1.00	42.50	SOLV
HETATM 3060	OH2 WAT D	52	6.494	33.164	51.420	1.00	40.65	SOLV
HETATM 3061	OH2 WAT D	53	24.913	44.799	72.298	1.00	17.10	SOLV
HETATM 3062	OH2 WAT D	54	51.156	35.095	48.814	1.00	23.05	SOLV
HETATM 3063	OH2 WAT D	55	16.518	41.750	45.596	1.00	49.25	SOLV
HETATM 3064	OH2 WAT D	56	10.326	16.413	61.267	1.00	46.03	SOLV
HETATM 3065	OH2 WAT D	57	25.316	47.708	73.062	1.00	22.73	SOLV
HETATM 3066	OH2 WAT D	58	4.013	33.865	76.173	1.00	44.82	SOLV
HETATM 3067	OH2 WAT D	59	24.846	18.072	36.805	1.00	34.67	SOLV
HETATM 3068	OH2 WAT D	60	15.930	56.853	61.737	1.00	55.56	SOLV
HETATM 3069	OH2 WAT D	61	49.662	44.249	48.982	1.00	28.72	SOLV
HETATM 3070	OH2 WAT D	62	23.232	17.421	53.920	1.00	13.11	SOLV
HETATM 3071	OH2 WAT D	63	39.293	23.035	33.289	1.00	35.79	SOLV
HETATM 3072	OH2 WAT D	64	19.908	20.169	44.339	1.00	24.33	SOLV
HETATM 3073	OH2 WAT D	65	33.259	21.655	69.560	1.00	45.10	SOLV
HETATM 3074	OH2 WAT D	66	27.528	53.947	68.629	1.00	44.79	SOLV
HETATM 3075	OH2 WAT D	67	18.774	48.716	52.865	1.00	54.01	SOLV
HETATM 3076	OH2 WAT D	68	10.877	29.062	63.401	1.00	27.08	SOLV
HETATM 3077	OH2 WAT D	69	43.057	31.367	28.786	1.00	30.16	SOLV
HETATM 3078	OH2 WAT D	70	24.816	44.057	43.447	1.00	20.11	SOLV
HETATM 3079	OH2 WAT D	71	37.368	38.823	46.381	1.00	33.55	SOLV
HETATM 3080	OH2 WAT D	72	9.038	18.327	63.519	1.00	31.34	SOLV
HETATM 3081	OH2 WAT D	73	51.799	20.829	65.265	1.00	28.32	SOLV
HETATM 3082	OH2 WAT D	74	17.556	58.515	57.254	1.00	19.27	SOLV
HETATM 3083	OH2 WAT D	75	28.436	27.904	79.425	1.00	27.13	SOLV
HETATM 3084	OH2 WAT D	76	18.939	35.798	35.800	1.00	94.18	SOLV
HETATM 3085	OH2 WAT D	77	34.359	31.251	46.688	1.00	73.70	SOLV
HETATM 3086	OH2 WAT D	78	44.373	51.649	60.029	1.00	30.23	SOLV
HETATM 3087	OH2 WAT D	79	28.537	63.478	48.324	1.00	21.09	SOLV
HETATM 3088	OH2 WAT D	80	6.869	44.113	72.030	1.00	28.59	SOLV
HETATM 3089	OH2 WAT D	81	42.882	18.761	71.115	1.00	31.80	SOLV
HETATM 3090	OH2 WAT D	82	36.712	59.078	53.901	1.00	40.11	SOLV
HETATM 3091	OH2 WAT D	83	37.506	42.495	40.104	1.00	51.37	SOLV
HETATM 3092	OH2 WAT D	84	40.054	38.439	55.415	1.00	20.07	SOLV
HETATM 3093	OH2 WAT D	85	32.170	56.633	72.920	1.00	45.23	SOLV
HETATM 3094	OH2 WAT D	86	24.470	53.877	47.119	1.00	41.18	SOLV
HETATM 3095	OH2 WAT D	87	48.585	35.663	67.518	1.00	33.40	SOLV
HETATM 3096	OH2 WAT D	88	29.541	57.166	42.788	1.00	44.61	SOLV
HETATM 3097	OH2 WAT D	89	47.814	28.707	41.228	1.00	45.64	SOLV
HETATM 3098	OH2 WAT D	90	49.377	52.112	63.320	1.00	22.26	SOLV
HETATM 3099	OH2 WAT D	91	44.219	43.589	43.912	1.00	39.90	SOLV
HETATM 3100	OH2 WAT D	92	25.913	61.639	75.382	1.00	48.28	SOLV
HETATM 3101	OH2 WAT D	93	8.623	30.749	49.707	1.00	40.37	SOLV
HETATM 3102	OH2 WAT D	94	45.634	41.080	40.990	1.00	21.46	SOLV

Figure 19-48

HETATM	3103	OH2	WAT	D	95	29.984	34.886	51.725	1.00	35.75	SOLV
HETATM	3104	OH2	WAT	D	96	13.051	21.934	49.804	1.00	46.73	SOLV
HETATM	3105	OH2	WAT	D	97	32.412	65.913	55.822	1.00	43.39	SOLV
HETATM	3106	OH2	WAT	D	98	35.056	43.390	38.348	1.00	34.53	SOLV
HETATM	3107	OH2	WAT	D	99	22.360	47.680	60.688	1.00	19.16	SOLV
HETATM	3108	OH2	WAT	D	100	50.755	19.722	57.906	1.00	42.45	SOLV
HETATM	3109	OH2	WAT	D	101	7.875	37.690	74.094	1.00	37.18	SOLV
HETATM	3110	OH2	WAT	D	102	24.080	26.796	43.617	1.00	30.72	SOLV
HETATM	3111	OH2	WAT	D	103	45.206	34.126	75.765	1.00	39.89	SOLV
HETATM	3112	OH2	WAT	D	104	26.110	54.786	40.685	1.00	29.58	SOLV
HETATM	3113	OH2	WAT	D	105	25.918	39.658	77.647	1.00	44.04	SOLV
HETATM	3114	OH2	WAT	D	106	41.578	18.191	36.809	1.00	42.22	SOLV
HETATM	3115	OH2	WAT	D	107	31.945	51.420	73.896	1.00	41.15	SOLV
HETATM	3116	OH2	WAT	D	108	16.722	60.311	51.182	1.00	48.74	SOLV
HETATM	3117	OH2	WAT	D	109	43.604	38.573	78.141	1.00	36.22	SOLV
HETATM	3118	OH2	WAT	D	110	16.063	15.496	69.430	1.00	55.36	SOLV
HETATM	3119	OH2	WAT	D	111	21.630	22.785	49.145	1.00	36.52	SOLV
HETATM	3120	OH2	WAT	D	112	27.479	56.647	44.026	1.00	50.82	SOLV
HETATM	3121	OH2	WAT	D	113	14.739	51.674	61.674	1.00	35.55	SOLV
HETATM	3122	OH2	WAT	D	114	50.063	26.435	54.358	1.00	50.86	SOLV
HETATM	3123	OH2	WAT	D	115	43.935	38.427	73.129	1.00	44.21	SOLV
HETATM	3124	OH2	WAT	D	116	49.707	31.478	57.709	1.00	36.11	SOLV
HETATM	3125	OH2	WAT	D	117	25.032	43.463	55.676	1.00	38.06	SOLV
HETATM	3126	OH2	WAT	D	118	10.618	46.623	59.838	1.00	26.33	SOLV
HETATM	3127	OH2	WAT	D	119	48.466	33.382	61.437	1.00	19.82	SOLV
HETATM	3128	OH2	WAT	D	120	44.157	40.058	37.907	1.00	42.95	SOLV
HETATM	3129	OH2	WAT	D	121	51.267	29.446	52.889	1.00	38.93	SOLV
HETATM	3130	OH2	WAT	D	122	16.653	15.228	72.975	1.00	45.41	SOLV
HETATM	3131	OH2	WAT	D	123	36.898	45.148	41.936	1.00	27.00	SOLV
HETATM	3132	OH2	WAT	D	124	49.655	34.591	59.117	1.00	38.97	SOLV
HETATM	3133	OH2	WAT	D	125	12.285	57.594	42.107	1.00	23.56	SOLV
HETATM	3134	OH2	WAT	D	126	28.294	57.644	73.289	1.00	34.79	SOLV
HETATM	3135	OH2	WAT	D	127	19.138	60.403	61.551	1.00	28.58	SOLV
HETATM	3136	OH2	WAT	D	128	30.300	33.685	34.047	1.00	27.37	SOLV
HETATM	3137	OH2	WAT	D	129	40.898	53.983	47.254	1.00	16.30	SOLV
HETATM	3138	OH2	WAT	D	130	43.550	32.160	38.272	1.00	38.86	SOLV
HETATM	3139	OH2	WAT	D	131	18.624	13.959	56.194	1.00	37.70	SOLV
HETATM	3140	OH2	WAT	D	132	18.580	12.901	62.894	1.00	27.28	SOLV
HETATM	3141	OH2	WAT	D	133	35.830	30.296	50.621	1.00	42.47	SOLV
HETATM	3142	OH2	WAT	D	134	51.219	35.855	51.878	1.00	20.37	SOLV
HETATM	3143	OH2	WAT	D	135	50.428	22.486	49.267	1.00	39.37	SOLV
HETATM	3144	OH2	WAT	D	136	51.633	29.369	63.918	1.00	33.99	SOLV
HETATM	3145	OH2	WAT	D	137	46.384	43.924	55.825	1.00	22.63	SOLV
HETATM	3146	OH2	WAT	D	138	30.356	25.767	28.762	1.00	25.84	SOLV
HETATM	3147	OH2	WAT	D	139	25.070	47.842	60.819	1.00	25.00	SOLV
HETATM	3148	OH2	WAT	D	140	47.097	49.394	69.367	1.00	30.58	SOLV
HETATM	3149	OH2	WAT	D	141	15.246	37.581	73.398	1.00	36.82	SOLV
HETATM	3150	OH2	WAT	D	142	8.341	23.099	64.695	1.00	35.89	SOLV
HETATM	3151	OH2	WAT	D	143	30.065	18.220	46.048	1.00	14.26	SOLV
HETATM	3152	OH2	WAT	D	144	11.930	46.453	57.606	1.00	36.15	SOLV

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US00/24700

A. CLASSIFICATION OF SUBJECT MATTER

IPC(7) :C07K 14/00; G01N 53/573

US CL :Please See Extra Sheet.

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : Please See Extra Sheet.

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

Please See Extra Sheet.

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	KAKUTA et al. Crystal Structure of the Sulfotransferase Domain of Human Heparan Sulfate N-Deacetylase/N-Sulfotransferase 1. The Journal of Biological Chemistry. 16 April 1999, Volume 274, Number 16, pages 10673-10676, see especially the abstract.	1-19
Y	SUEYOSHI et al. A role of Lys-614 in the sulfotransferase activity of human heparan sulfate N-deacetylase/N-sulfotransferase. FEBS Letters. 1998, Volume 433, pages 211-214, see especially the abstract.	1-19

☒ Further documents are listed in the continuation of Box C. ☐ See patent family annex.

* Special categories of cited documents:	*T	later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
A document defining the general state of the art which is not considered to be of particular relevance	*X*	document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
E earlier document published on or after the international filing date	*Y*	document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
L document which may throw doubt on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	*A*	document member of the same patent family
O document referring to an oral disclosure, use, exhibition or other means		
P document published prior to the international filing date but later than the priority date claimed		

Date of the actual completion of the international search 29 DECEMBER 2000	Date of mailing of the international search report 25 JAN 2001
Name and mailing address of the ISA/US Commissioner of Patents and Trademarks Box PCT Washington, D.C. 20231 Facsimile No. (703) 305-3830	Authorized officer ARDIN MARCHEL Telephone No. (703) 308-0196

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US00/24700

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	AHMAD et al. WD Repeats of the p48 Subunit of Chicken Chromatin Assembly Factor-1 Required for in Vitro Interaction with Chicken Histone Deacetylase-2. The Journal of Biological Chemistry. 04 June 1999, Volume 274, Number 23, pages 16646-16653, see especially the abstract.	1-19
Y	JOHN et al. Rhizobium NodB protein involved in nodulation signal synthesis is a chitooligosaccharide deacetylase. Proceedings of the National Academy of Sciences, USA. January 1993, Volume 90, pages 625-629, see especially the abstract.	1-19
A	US 5,780,594 A (CARTER) 14 July 1998, see the entire disclosure.	1-19

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US00/24700

A. CLASSIFICATION OF SUBJECT MATTER:

US CL :

530/550 and 435/7.2

B. FIELDS SEARCHED

Minimum documentation searched

Classification System: U.S.

530/500,535,550; 435/8,7.2; 514/2

B. FIELDS SEARCHED

Electronic data bases consulted (Name of data base and where practicable terms used):

CAS, BIOTECH ABS, MEDLINE, EMBASE, WPI, WEST covering search terms: deacetylase, human, crystal, histone, inhibitor, x-ray, and crystallography

THIS PAGE BLANK (USPTO)